CoRe Optimizer

CLASS core_optimizer.CoRe(params, Ir=1e-3, $step_sizes=(1e-6$, 1e-2), etas=(0.7375, 1.2), betas=(0.7375, 0.8125, 250.0, 0.99), eps=1e-8, $weight_decay=0.1$, $score_history=0$, frozen=0.0, *, maximize=False, foreach=None)

Implements the Continual Resilient (CoRe) optimizer.

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input: \theta (params), f(\theta) (objective), s_{\min}, s_{\max} (step sizes),
               \eta_-, \eta_+ (etas), \beta_1^a, \beta_1^b, \beta_1^c, \beta_2 (betas), \epsilon (eps),
               d (weight decay), t_{\text{hist}} (score history), p_{\text{frozen}} (frozen)
initialize : s_0 \leftarrow \text{lr}, \ g_0 \leftarrow 0, \ h_0 \leftarrow 0, \ S_0 \leftarrow 0
for t=1 to \dots do
      G_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1})
      if maximize
            G_t \leftarrow -G_t
      \beta_{1,t} \leftarrow \beta_1^{\rm b} + (\beta_1^{\rm a} - \beta_1^{\rm b}) \exp\{-[(t-1)/\beta_1^{\rm c}]^2\}
      g_t \leftarrow \beta_{1,t} g_{t-1} + (1 - \beta_{1,t}) G_t
      if \beta_2 > 0
            h_t \leftarrow \beta_2 h_{t-1} + (1 - \beta_2) G_t^2
      P_t \leftarrow 1
      if t_{\text{hist}} > 0 \land t > t_{\text{hist}} \land S_{t-1} \text{ top-}p_{\text{frozen}} \text{ in } \mathbf{S}_{t-1}
            P_t \leftarrow 0
      if g_{t-1}g_tP_t > 0
            s_t \leftarrow \min(\eta_+ s_{t-1}, s_{\max})
      else if g_{t-1}g_tP_t < 0
            s_t \leftarrow \max(\eta_{-}s_{t-1}, s_{\min})
      else
            s_t \leftarrow s_{t-1}
      if \beta_2 > 0
            u_t \leftarrow g_t/(1-\beta_{1,t}^t)/\{[h_t/(1-\beta_2^t)]^{0.5}+\epsilon\}
      else
            u_t \leftarrow \operatorname{sgn}(g_t)
      if t_{\rm hist} > 0
            if t \leq t_{\text{hist}}
                  S_t \leftarrow S_{t-1} + t_{\text{hist}}^{-1} g_t u_t P_t s_t
            else
                 S_t \leftarrow (1 - t_{\text{hist}}^{-1}) S_{\varepsilon}^{\tau - 1} + t_{\text{hist}}^{-1} g_t u_t P_t s_t
      \theta_t \leftarrow (1 - d|u_t|P_t s_t)\theta_{t-1} - u_t P_t s_t
```

return θ_t

For further details regarding the algorithm we refer to the papers Lifelong Machine Learning Potentials and CoRe optimizer: an all-in-one solution for machine learning.

Parameters:

- params (iterable): iterable of parameters to optimize or dicts defining parameter groups
- **Ir** (float, optional): learning rate to set initial step size (default: 1e-3)
- **step_sizes** (*Tuple[float, float], optional*): pair of minimal and maximal allowed step sizes (recommendation: maximal step size of 1e-3 for mini-batch learning, 1.0 for batch learning, and 1e-2 for intermediate cases) (default: (1e-6, 1e-2))
- etas (*Tuple[float, float], optional*): pair of etaminus and etaplus that are multiplicative increase and decrease factors (default: (0.7375, 1.2))
- **betas** (*Tuple[float, float, float, float], optional*): coefficients beta1a, beta1b, beta1c, and beta2 used for computing running averages of gradient and its square (default: (0.7375, 0.8125, 250.0, 0.99))
- **eps** (*float, optional*): term added to the denominator to improve numerical stability (default: 1e-8)
- weight_decay (float or List[float], optional): weight decay for all parameters or list of weight decays for parameter groups (default: 0.1)
- score_history (int, optional): number of optimization steps to build the score history before applying plasticity factors (default: 0)
- **frozen** (*float or List[float], optional*): fraction of all parameters frozen by the plasticity factors or list of fractions for parameter groups (applies if score_history > 0) (default: 0.0)
- maximize (bool, optional): maximize the objective with respect to the params, instead of minimizing (default: False)
- **foreach** (bool, optional): whether foreach implementation of optimizer is used. If unspecified by the user (so foreach is None), we will try to use foreach over the for-loop implementation on CUDA, since it is usually significantly more performant. Note that the foreach implementation uses ~ sizeof(params) more peak memory than the for-loop version due to the intermediates being a tensorlist vs just one tensor. If memory is prohibitive, batch fewer parameters through the optimizer at a time or switch this flag to False (default: None)