

## Appendix A HMC-CVA Algorithm

We denote the original chain  $X$  and its corresponding control variate  $Y$  as  $X^+$  and  $Y^+$  for emphasis.

- 1: **procedure** HMC-CVA( $X_0^+, X_0^-, Y_0^+, n, T$ )
- 2: **for**  $i = 0$  to  $n - 1$  **do**
- 3:   Sample  $p_i^+ \sim \mathcal{N}(0, I_D)$ .
- 4:   Set  $p_i^- = -p_i^+$ .
- 5:   Set  $p'_i = p_i^+$ . ▷ Shared  $p_i$
- 6:   Set  $(q_{i+1}^+, p_{i+1}^+) = \Psi_{H,T}(X_i^+, p_i^+)$ .
- 7:   Set  $(q_{i+1}^-, p_{i+1}^-) = \Psi_{H,T}(X_i^-, p_i^-)$ .
- 8:   Set  $(q'_{i+1}, p'_{i+1}) = \Psi_{H',T}(Y_i^+, p'_i)$ .
- 9:   Sample  $b_i \sim \text{Unif}([0, 1])$ . ▷ Shared  $b_i$
- 10:   Set  $X_{i+1}^+ = \text{MHADJ}(X_i^+, q_{i+1}^+, p_i^+, p'_{i+1}, b_i, H)$ .
- 11:   Set  $X_{i+1}^- = \text{MHADJ}(X_i^-, q_{i+1}^-, p_i^-, p'_{i+1}, b_i, H)$ .
- 12:   Set  $Y_{i+1}^+ = \text{MHADJ}(Y_i^+, q'_{i+1}, p'_i, p'_{i+1}, b_i, H')$ .
- 13:   Set  $Y_{i+1}^- = 2\mu - Y_{i+1}^+$ .
- 14: **end for**
- 15:   Compute unbiased estimate  $\hat{\mathbb{E}}_Q[f(Y)]$ .
- 16:   Estimate optimal  $\beta$  by linear regression.
- 17: **for**  $i = 1$  to  $n$  **do**
- 18:   Set  $Z_{i,j}^+ = f_j(X_i^+) - \beta_j^\top (f(Y_i^+) - \hat{\mathbb{E}}_Q[f(Y)])$ .
- 19:   Set  $Z_{i,j}^- = f_j(X_i^-) - \beta_j^\top (f(Y_i^-) - \hat{\mathbb{E}}_Q[f(Y)])$ .
- 20:   Set  $Z_i = \frac{1}{2}(Z_i^+ + Z_i^-)$ .
- 21: **end for**
- 22: **end procedure**