A Appendix: Proof of Theorem 1

We first show that the estimate is unbiased. Indeed, for every $i \neq j$ we can rewrite $L(z)$ as $\mathbb{E}_\pi \ell_{\pi(i),\pi(j)}(z)$. Therefore,

$$L(z) = \frac{1}{k^2-k} \sum_{i \neq j \in [k]} L(z) = \frac{1}{k^2-k} \sum_{i \neq j \in [k]} \mathbb{E}_\pi \ell_{\pi(i),\pi(j)}(z) = \mathbb{E}_\pi L_\pi(z) \,,$$

which proves that the multibatch estimate is unbiased.

Next, we turn to analyze the variance of the multibatch estimate. let $I \subset [k]^4$ be all the indices i, j, s, t s.t. $i \neq j, s \neq t$, and we partition I to $I_1 \cup I_2 \cup I_3$, where I_1 is the set where $i = s$ and $j = t$, I_2 is when all indices are different, and I_3 is when $i = s$ and $j \neq t$ or $i \neq s$ and $j = t$. Then:

$$\mathbb{E}_\pi \|\nabla L_\pi(z) - \nabla L(z)\|^2 = \frac{1}{(k^2-k)^2} \mathbb{E}_\pi \sum_{(i,j,s,t) \in I} (\nabla \ell_{\pi(i),\pi(j)}(z) - \nabla L(z)) \cdot (\nabla \ell_{\pi(s),\pi(t)}(z) - \nabla L(z))$$

$$= \sum_{r=1}^{d} \frac{1}{(k^2-k)^2} \sum_{q=1}^{3} \sum_{(i,j,s,t) \in I_q} \mathbb{E}_\pi (\nabla_r \ell_{\pi(i),\pi(j)}(z) - \nabla_r L(z)) \, (\nabla_r \ell_{\pi(s),\pi(t)}(z) - \nabla_r L(z))$$

For every r, denote by $A^{(r)}$ the matrix with $A^{(r)}_{i,j} = \nabla_r \ell_{i,j}(z) - \nabla_r L(z)$. Observe that for every r, $\mathbb{E}_{i \neq j} A^{(r)}_{i,j} = 0$, and that

$$\sum_r \mathbb{E}_{i \neq j} (A^{(r)}_{i,j})^2 = \mathbb{E}_{i \neq j} \|\nabla \ell_{i,j}(z) - \nabla L(z)\|^2.$$

Therefore,

$$\mathbb{E}_\pi \|\nabla L_\pi(z) - \nabla L(z)\|^2 = \sum_{r=1}^{d} \frac{1}{(k^2-k)^2} \sum_{q=1}^{3} \sum_{(i,j,s,t) \in I_q} \mathbb{E}_\pi A^{(r)}_{\pi(i),\pi(j)} A^{(r)}_{\pi(s),\pi(t)}$$

Let us momentarily fix r and omit the superscript from $A^{(r)}$. We consider the value of $\mathbb{E}_\pi A_{\pi(i),\pi(j)} A_{\pi(s),\pi(t)}$ according to the value of q.

- For $q = 1$: we obtain $\mathbb{E}_\pi A^2_{\pi(i),\pi(j)}$ which is the variance of the random variable $\nabla_r \ell_{i,j}(z) - \nabla_r L(z)$.
- For $q = 2$: When we fix i, j, s, t which are all different, and take expectation over π, then all products of off-diagonal elements of A appear the same number of times in $\mathbb{E}_\pi A_{\pi(i),\pi(j)} A_{\pi(s),\pi(t)}$. Therefore, this quantity is proportional to $\sum_{p \neq r} v_p v_r$, where v is the vector of all non-diagonal entries of A. Since $\sum_p v_p = 0$, we obtain (using Lemma 1) that $\sum_{p \neq r} v_p v_r \leq 0$, which means that the entire sum for this case is non-positive.
- For $q = 3$: Let us consider the case when $i = s$ and $j \neq t$, and the derivation for the case when $i \neq s$ and $j = t$ is analogous. The expression we obtain is $\mathbb{E}_\pi A_{\pi(i),\pi(j)} A_{\pi(i),\pi(t)}$. This is like first sampling a row and then sampling, without replacement, two indices from the row (while not allowing to take the diagonal element). So, we can rewrite the expression as:

$$\begin{aligned} \mathbb{E}_\pi A_{\pi(i),\pi(j)} A_{\pi(s),\pi(t)} &= \mathbb{E}_{i \sim [m]} \mathbb{E}_{j,t \in [m] \setminus \{i\} : j \neq t} A_{i,j} A_{i,t} \\ &\leq \mathbb{E}_{i \sim [m]} \left(\mathbb{E}_{j \neq i} A_{i,j} \right)^2 = \mathbb{E}_{i \sim [m]} (\bar{A}_i)^2 \,, \end{aligned} \tag{5}$$

  where we denote $\bar{A}_i = \mathbb{E}_{j \neq i} A_{i,j}$ and in the inequality we used again Lemma 1.

Finally, the bound on the variance follows by observing that the number of summands in I_1 is $k^2 - k$ and the number of summands in I_3 is $O(k^3)$. This concludes our proof.

Lemma 1 *Let $v \in \mathbb{R}^n$ be any vector. Then,*

$$\mathop{\mathbb{E}}_{s \neq t}[v_s v_t] \leq (\mathop{\mathbb{E}}_{i}[v_i])^2$$

In particular, if $\mathbb{E}_i[v_i] = 0$ then $\sum_{s \neq t} v_s v_t \leq 0$.

Proof For simplicity, we use $\mathbb{E}[v]$ for $\mathbb{E}_i[v_i]$ and $\mathbb{E}[v^2]$ for $\mathbb{E}_i[v_i^2]$. Then:

$$\begin{aligned}
\mathop{\mathbb{E}}_{s \neq t} v_s v_t &= \frac{1}{n^2 - n} \sum_{s=1}^{n} \sum_{t=1}^{n} v_s v_t - \frac{1}{n^2 - n} \sum_{s=1}^{n} v_s^2 \\
&= \frac{1}{n^2 - n} \sum_{s=1}^{n} v_s \sum_{t=1}^{n} v_t - \frac{1}{n^2 - n} \sum_{s=1}^{n} v_s^2 \\
&= \frac{n^2}{n^2 - n} \mathbb{E}[v]^2 - \frac{n}{n^2 - n} \mathbb{E}[v^2] \\
&= \frac{n}{n^2 - n} (\mathbb{E}[v]^2 - \mathbb{E}[v^2]) + \frac{n^2 - n}{n^2 - n} \mathbb{E}[v]^2 \\
&\leq 0 + \mathbb{E}[v]^2
\end{aligned}$$

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