Supplementary for Provably Optimal Algorithms for Generalized Linear Contextual Bandits

A. Proof of Theorem 1

In the following, for simplicity, we will drop the subscript n when there is no ambiguity. Therefore, V_n is denoted V and so on.

To prove normality-type results of the maximum likelihood estimator $\hat{\theta}$, typically we first show the $n^{-1/2}$ -consistency of $\hat{\theta}$ to θ^* . Then, by using a second-order Taylor expansion or Newton-step, we can prove the desired normality of $\hat{\theta}$. More details can be found in standard textbooks such as Van der Vaart (2000).

Since m is twice differentiable with $\ddot{m} \ge 0$, the maximum-likelihood estimation can be written as the solution to the following equation

$$\sum_{i=1}^{n} (Y_i - \mu(X'_i\theta)) X_i = 0.$$
(15)

Define $G(\theta) := \sum_{i=1}^{n} (\mu(X'_i\theta) - \mu(X'_i\theta^*)) X_i$, and we have

$$G(\theta^*) = 0 \text{ and } G(\hat{\theta}) = \sum_{i=1}^n \epsilon_i X_i ,$$
 (16)

where the noise ϵ_i is defined in (1). For convenience, define $Z := G(\hat{\theta}) = \sum_{i=1}^n \epsilon_i X_i$.

Step 1: Consistency of $\hat{\theta}$. We first prove the consistency of $\hat{\theta}$. For any $\theta_1, \theta_2 \in \mathbb{R}^d$, mean value theorem implies that there exists some $\bar{\theta} = v\theta_1 + (1-v)\theta_2$ with 0 < v < 1, such that

$$G(\theta_1) - G(\theta_2) = \left[\sum_{i=1}^n \dot{\mu}(X'_i\bar{\theta})X_iX'_i\right](\theta_1 - \theta_2) := F(\bar{\theta})(\theta_1 - \theta_2)$$
(17)

Since $\dot{\mu} > 0$ and $\lambda_{\min}(V) > 0$, we have

$$(\theta_1 - \theta_2)'(G(\theta_1) - G(\theta_2)) \ge (\theta_1 - \theta_2)'(\kappa V)(\theta_1 - \theta_2) > 0$$

for any $\theta_1 \neq \theta_2$. Hence, $G(\theta)$ is an injection from \mathbb{R}^d to \mathbb{R}^d , and so G^{-1} is a well-defined function. Consequently, (15) has a unique solution $\hat{\theta} = G^{-1}(Z)$.

Let us consider an η -neighborhood of θ^* , $\mathbb{B}_{\eta} := \{\theta : \|\theta - \theta^*\| \le \eta\}$, where $\eta > 0$ is a constant that will be specified later. Note that \mathcal{B}_{η} is a convex set, thus $\bar{\theta} \in \mathcal{B}_{\eta}$ as long as $\theta_1, \theta_2 \in \mathbb{B}_{\eta}$. Define $\kappa_{\eta} := \inf_{\theta \in \mathbb{B}_{\eta}} \dot{\mu}(x'\theta) > 0$. From (17), for any $\theta \in \mathcal{B}_{\eta}$,

$$\begin{split} \|G(\theta)\|_{V^{-1}}^2 &= \|G(\theta) - G(\theta^*)\|_{V^{-1}}^2 \\ &= (\theta - \theta^*)'F(\bar{\theta})V^{-1}F(\bar{\theta})(\theta - \theta^*) \\ &\geq \kappa_\eta^2 \lambda_{\min}(V) \|\theta - \theta^*\|^2 \,, \end{split}$$

where the last inequality is due to the fact that $F(\bar{\theta}) \succeq \kappa_{\eta} V$.

On the other hand, Lemma A of Chen et al. (1999) implies that

$$\left\{\theta : \|G(\theta)\|_{V^{-1}} \le \kappa_\eta \eta \sqrt{\lambda_{\min}(V)}\right\} \subset \mathcal{B}_\eta.$$

Now it remains to upper bound $||Z||_{V^{-1}} = ||G(\hat{\theta})||_{V^{-1}}$ to ensure $\hat{\theta} \in \mathbb{B}_{\eta}$. To do so, we need the following technical lemma, whose proof is deferred to Section C.

Lemma 7. Recall σ which is the constant in (2). For any $\delta > 0$, define the following event:

$$\mathcal{E}_G := \left\{ \|Z\|_{V^{-1}} \le 4\sigma \sqrt{d + \log(1/\delta)} \right\} \,.$$

Then, \mathcal{E}_G holds with probability at least $1 - \delta$.

Suppose \mathcal{E}_G holds for the rest of the proof. Then, $\eta \geq \frac{4\sigma}{\kappa_\eta} \sqrt{\frac{d + \log(1/\delta)}{\lambda_{\min}(V)}}$ implies $\left\| \hat{\theta}_t - \theta \right\| \leq \eta$. Since $\kappa = \kappa_1$, we have $\kappa_\eta \geq \kappa$ as long as $\eta \leq 1$. Thus, we have

$$\left\|\hat{\theta} - \theta\right\| \le \frac{4\sigma}{\kappa} \sqrt{\frac{d + \log(1/\delta)}{\lambda_{\min}(V)}} \le 1,$$
(18)

when $\lambda_{\min}(V) \ge 16\sigma^2 \left[d + \log(1/\delta)\right]/\kappa^2$.

Step 2: Normality of $\hat{\theta}$. Now, we are ready to precede to prove the normality result. The following assumes \mathcal{E}_G holds (which is high-probability event, according to Lemma 7).

Define $\Delta := \hat{\theta} - \theta^*$. It follows from (17) that there exists a $v \in [0, 1]$ such that

$$Z = G(\hat{\theta}) - G(\theta^*) = (H + E)\Delta_{\theta}$$

where $\tilde{\theta} := v\theta^* + (1-v)\hat{\theta}$, $H := F(\theta^*) = \sum_{i=1}^n \dot{\mu}(X'_i\theta^*)X_iX'_i$ and $E := F(\tilde{\theta}) - F(\theta^*)$. Intuitively, when $\hat{\theta}$ and θ^* are close, elements in E are small. By the mean value theorem,

$$E = \sum_{i=1}^{n} \left(\dot{\mu}(X_i'\tilde{\theta}) - \dot{\mu}(X_i'\theta^*) \right) X_i X_i' = \sum_{i=1}^{n} \ddot{\mu}(r_i) X_i' \Delta X_i X_i'$$

for some $r_i \in \mathbb{R}$. Since $\ddot{\mu} \leq M_{\mu}$ and $v \in [0, 1]$, for any $x \in \mathbb{R}^d \setminus \{\mathbf{0}\}$, we have

$$\begin{aligned} x'H^{-1/2}EH^{-1/2}x &= (1-v)\sum_{i=1}^{n}\ddot{\mu}(r_{i})X'_{i}\Delta \left\|x'H^{-1/2}X_{i}\right\|^{2} \\ &\leq \sum_{i=1}^{n}M_{\mu} \|X_{i}\| \|\Delta\| \left\|x'H^{-1/2}X_{i}\right\|^{2} \\ &\leq M_{\mu} \|\Delta\| \left(x'H^{-1/2}\left(\sum_{i=1}^{n}X_{i}X'_{i}\right)H^{-1/2}x\right) \\ &\leq \frac{M_{\mu}}{\kappa} \|\Delta\| \|x\|^{2}, \end{aligned}$$

where we have used the assumption that $||X_i|| \leq 1$ for the second inequality. Therefore,

$$\left\| H^{-1/2} E H^{-1/2} \right\| \le \frac{M_{\mu}}{\kappa} \left\| \Delta \right\| \le \frac{4M_{\mu}\sigma}{\kappa^2} \sqrt{\frac{d + \log(1/\delta)}{\lambda_{\min}(V)}} \,. \tag{19}$$

When $\lambda_{\min}(V) \ge 64M_{\mu}^2\sigma^2(d+\log(1/\delta))/\kappa^4$, we have

$$\left\| H^{-1/2} E H^{-1/2} \right\| \le 1/2.$$
 (20)

Now we are ready to prove the theorem. For any $x \in \mathbb{R}^d$,

$$x'(\hat{\theta} - \theta^*) = x'(H + E)^{-1}Z = x'H^{-1}Z - x'H^{-1}E(H + E)^{-1}Z.$$
(21)

Note that the matrix (H + E) is nonsingular, so its inversion exists.

For the first term, $\{\epsilon_i\}$ are sub-Gaussian random variables with sub-Gaussian parameter σ . Define

$$D := [X_1, X_2, \dots, X_n]' \in \mathbb{R}^{n \times d}$$

to be the design matrix. Hoeffding inequality gives

$$\mathbb{P}\{|x'H^{-1}Z| \ge t\} \le 2\exp\left\{-\frac{t^2}{2\sigma^2 \|x'H^{-1}D'\|^2}\right\}.$$
(22)

Since $H \succeq \kappa V = \kappa D'D$, we have

$$\left\| x'H^{-1}D' \right\|^2 = x'H^{-1}D'DH^{-1}x \le \frac{1}{\kappa^2}x'V^{-1}x = \frac{1}{\kappa^2}\left\| x \right\|_{V^{-1}}^2,$$

so (22) implies

$$\mathbb{P}\{|x'H^{-1}Z| \ge t\} \le 2\exp\left\{-\frac{t^2\kappa^2}{2\sigma^2 \|x\|_{V^{-1}}^2}\right\}.$$

Let the right-hand side be 2δ and solve for t, we obtain that with probability at least $1 - 2\delta$,

$$|x'H^{-1}Z| \le \frac{\sqrt{2}\sigma}{\kappa} \sqrt{\log(1/\delta)} \, \|x\|_{V^{-1}} \,.$$
(23)

For the second term,

$$\begin{aligned} |x'H^{-1}E(H+E)^{-1}Z| &\leq ||x||_{H^{-1}} \left\| H^{-1/2}E(H+E)^{-1}Z \right\| \\ &\leq ||x||_{H^{-1}} \left\| H^{-1/2}E(H+E)^{-1}H^{1/2} \right\| ||Z||_{H^{-1}} \\ &\leq \frac{1}{\kappa} ||x||_{V^{-1}} \left\| H^{-1/2}E(H+E)^{-1}H^{1/2} \right\| ||Z||_{V^{-1}} , \end{aligned}$$
(24)

where the last inequality is due to the fact that $H \succeq \kappa V$. Since $(H + E)^{-1} = H^{-1} - H^{-1}E(H + E)^{-1}$, we have

$$\begin{split} \left\| H^{-1/2} E(H+E)^{-1} H^{1/2} \right\| &= \left\| H^{-1/2} E\left(H^{-1} - H^{-1} E(H+E)^{-1} \right) H^{1/2} \right\| \\ &= \left\| H^{-1/2} E H^{-1/2} + H^{-1/2} E H^{-1} E(H+E)^{-1} H^{1/2} \right\| \\ &\leq \left\| H^{-1/2} E H^{-1/2} \right\| + \left\| H^{-1/2} E H^{-1/2} \right\| \left\| H^{-1/2} E(H+E)^{-1} H^{1/2} \right\| \,. \end{split}$$

By solving this inequality, we get

$$\left\| H^{-1/2} E(H+E)^{-1} H^{1/2} \right\| \le \frac{\left\| H^{-1/2} E H^{-1/2} \right\|}{1 - \left\| H^{-1/2} E H^{-1/2} \right\|} \le 2 \left\| H^{-1/2} E H^{-1/2} \right\| \le \frac{8M_{\mu}\sigma}{\kappa^2} \sqrt{\frac{d + \log(1/\delta)}{\lambda_{\min}(V)}} + \frac{1}{2} \left\| H^{-1/2} E H^{-1/2} \right\| \le \frac{1}{2} \left\| H^{-1/2} E H^{-1/2} \right\|$$

where we have used (20) and (19) in the second and third inequalities, respectively. Combining it with (24) and the bound in \mathcal{E}_G , we have

$$|x'H^{-1}E(H+E)^{-1}Z| \leq \frac{32M_{\mu}\sigma^2}{\kappa^3} \frac{d + \log(1/\delta)}{\sqrt{\lambda_{\min}(V)}} \|x\|_{V^{-1}}.$$
(25)

From (21), (23) and (25), one can see that (5) holds as long as the lower bound (4) for $\lambda_{\min}(V)$ holds. Finally, an application of a union bound on two small-probability events (given in Lemma 7 and (23), respectively) asserts that (5) holds with probability at least $1 - 3\delta$.

B. Proof of Proposition 1

In the following, for simplicity, we will drop the subscript n when there is no ambiguity. Therefore, V_n is denoted V and so on.

Let X be a random vector drawn from the distribution ν . Define $Z := \Sigma^{-1/2} X$. Then Z is isotropic, namely, $\mathbb{E}[ZZ'] = \mathbf{I}_d$. Define $U = \sum_{t=1}^n Z_t Z'_t = \Sigma^{-1/2} V \Sigma^{-1/2}$. From Lemma 1, we have that, for any t, with probability at least $1 - 2 \exp(-C_2 t^2)$,

$$\lambda_{\min}(U) \ge n - C_1 \sigma^2 \sqrt{nd} - \sigma^2 t \sqrt{n}.$$

where σ is the sub-Gaussian parameter of Z, which is upper-bounded by $\|\Sigma^{-1/2}\| = \lambda_{\min}^{-1/2}(\Sigma)$ (see, e.g., Vershynin (2012)). We thus can rewrite the above inequality (which holds with probability $1 - \delta$ as

$$\lambda_{\min}(U) \ge n - \lambda_{\min}^{-1}(\Sigma) \left(C_1 \sigma^2 \sqrt{nd} + t \sqrt{n} \right)$$

We now bound the minimum eigenvalue of V, as follows:

$$\begin{aligned} \lambda_{\min}(V) &= \min_{x \in \mathbb{B}^d} x' V x \\ &= \min_{x \in \mathbb{B}^d} x' \Sigma^{1/2} U \Sigma^{1/2} x \\ &\geq \lambda_{\min}(U) \min_{x \in \mathbb{B}^d} x' \Sigma x \\ &= \lambda_{\min}(U) \lambda_{\min}(\Sigma) \\ &\geq \lambda_{\min}(\Sigma) \left(n - \lambda_{\min}^{-1}(\Sigma) (C_1 \sigma^2 \sqrt{nd} + t \sqrt{n}) \right) \\ &= \lambda_{\min}(\Sigma) n - C_1 \sqrt{nd} - C_2 \sqrt{n \log(1/\delta)} \,. \end{aligned}$$

Finally, it can be verified (Lemma 9) that the last expression above is no less than B as long as

$$n \ge \left(\frac{C_1\sqrt{d} + C_2\sqrt{\log(1/\delta)}}{\lambda_{\min}(\Sigma)}\right)^2 + \frac{2B}{\lambda_{\min}(\Sigma)},$$

finishing the proof.

C. Technical Lemmas and Proofs

C.1. Proof of Lemma 7

Noting that

$$||Z||_{V^{-1}} = ||V^{-1/2}Z||_2 = \sup_{||a||_2 \le 1} \langle a, V^{-1/2}Z \rangle,$$

let $\hat{\mathbb{B}}$ be a 1/2-net of the unit ball \mathbb{B}^d . Then $|\hat{\mathbb{B}}| \leq 6^d$ (Pollard, 1990, Lemma 4.1), and for any $x \in \mathbb{B}^d$, there is a $\hat{x} \in \hat{\mathbb{B}}$ such that $||x - \hat{x}|| \leq 1/2$. Consequently,

$$\begin{aligned} \langle x, V^{-1/2}Z \rangle &= \langle \hat{x}, V^{-1/2}Z \rangle + \langle x - \hat{x}, V^{-1/2}Z \rangle \\ &= \langle \hat{x}, V^{-1/2}Z \rangle + \|x - \hat{x}\| \left\langle \frac{x - \hat{x}}{\|x - \hat{x}\|}, V^{-1/2}Z \right\rangle \\ &\leq \langle \hat{x}, V^{-1/2}Z \rangle + \frac{1}{2} \sup_{z \in \mathbb{B}^d} \langle z, V^{-1/2}Z \rangle. \end{aligned}$$

Taking supremum on both sides, we get

$$\sup_{x \in \mathbb{B}^d} \langle x, V^{-1/2} Z \rangle \le 2 \max_{\hat{x} \in \hat{\mathbb{B}}} \langle \hat{x}, V^{-1/2} Z \rangle$$

Then a union bound argument implies

$$\begin{aligned} \mathbb{P}\left\{\|Z\|_{V^{-1}} > t\right\} &\leq \mathbb{P}\left\{\max_{\hat{x}\in\hat{\mathbb{B}}}\langle\hat{x}, V^{-1/2}Z\rangle > t/2\right\} \\ &\leq \sum_{\hat{x}\in\hat{\mathbb{B}}}\mathbb{P}\left\{\langle\hat{x}, V^{-1/2}Z\rangle > t/2\right\} \\ &\leq \sum_{\hat{x}\in\hat{\mathbb{B}}}\exp\left\{-\frac{t^2}{8\sigma^2 \left\|\hat{x}'V^{-1/2}X'\right\|^2}\right\} \\ &\leq \exp\left\{-t^2/(8\sigma^2) + d\log 6\right\},\end{aligned}$$

where we have used Hoeffding's inequality for the third inequality and $|\hat{\mathbb{B}}| \leq 6^d$ for the last inequality. A choice of $t = 4\sigma \sqrt{d + \log(1/\delta)}$ completes the proof.

C.2. Proof of Lemma 2

By Abbasi-Yadkori et al. (2011, Lemma 11), we have

$$\sum_{t=m+1}^{m+n} \|X_t\|_{V_t^{-1}}^2 \le 2\log \frac{\det V_{m+n+1}}{\det V_{m+1}} \le 2d\log\left(\frac{\operatorname{tr}(V_{m+1})+n}{d}\right) - 2\log \det V_{m+1}$$

Note that tr $(V_{m+1}) = \sum_{t=1}^{m} \text{tr} (X_t X'_t) = \sum_{t=1}^{m} ||X_t||^2 \le m$ and that $\det V_{m+1} = \prod_{i=1}^{d} \lambda_i \ge \lambda_{\min}^d(V_{m+1}) \ge 1$, where $\{\lambda_i\}$ are the eigenvalues of V_{m+1} . Applying Cauchy-Schwartz inequality yields

$$\sum_{t=m+1}^{m+n} \|X_t\|_{V_t^{-1}} \le \sqrt{n \sum_{t=m+1}^{m+n} \|X_t\|_{V_t^{-1}}^2} \le \sqrt{2nd \log\left(\frac{n+m}{d}\right)}.$$

C.3. Proof of Lemma 3

Define $G_t(\theta) = \sum_{i=1}^{t-1} (\mu(X'_i\theta) - \mu(X'_i\theta^*))X_i$ and $Z_t = \sum_{i=1}^{t-1} \epsilon_i X_i$. Following the same argument as in the proof of Theorem 1, we have $G_t(\hat{\theta}_t) = Z_t$ and

$$\|G_t(\theta)\|_{V_t^{-1}}^2 \ge \kappa^2 \|\theta - \theta^*\|_{V_t}^2$$
(26)

for any $\theta \in \{\theta : \|\theta - \theta^*\| \le 1\}$. Combining (26) with the following lemma and the equality $Z_t = G_t(\hat{\theta}_t)$ completes the proof.

Lemma 8. Suppose there is an integer m such that $\lambda_{\min}(V_m) \ge 1$, then for any $\delta \in (0, 1)$, with probability at least $1 - \delta$, for all t > m,

$$\|Z_t\|_{V_t^{-1}}^2 \le 4\sigma^2 \left(\frac{d}{2}\log(1+2t/d) + \log(1/\delta)\right).$$

Proof. For convenience, fix t such that t > m, and denote V_t and Z_t by V and Z, respectively. Furthermore, define $\overline{V} := V + \lambda I$ and let 1 be the vector of all 1s. It is easy to observe that

$$\|Z\|_{V^{-1}}^2 = \|Z\|_{\bar{V}^{-1}}^2 + Z'(V^{-1} - \bar{V}^{-1})Z.$$
⁽²⁷⁾

We start with bounding the second term. The ShermanMorrison formula gives

$$\bar{V}^{-1} = V^{-1} - \frac{\lambda V^{-2}}{1 + \lambda \mathbf{1}' V^{-1} \mathbf{1}}.$$

Since $\mathbf{1}'V^{-1}\mathbf{1} \ge 0$, the above implies that

$$\begin{array}{rcl}
0 &\leq& Z'(V^{-1}-\bar{V}^{-1})Z \\
&\leq& \lambda Z'V^{-2}Z \\
&\leq& \lambda \|V^{-1}\| \|Z\|_{V^{-1}}^2 \\
&=& \frac{\lambda}{\lambda_{\min}(V)} \|Z\|_{V^{-1}}^2 .
\end{array}$$

Since $\lambda_{\min}(V) \ge \lambda_{\min}(V_m) \ge 1$, we now have

$$0 \le Z'(V^{-1} - \bar{V}^{-1})Z \le \lambda \|Z\|_{V^{-1}}^2.$$

The above inequality together with (27) implies that

$$||Z||_{V^{-1}}^2 \le (1-\lambda)^{-1} ||Z||_{\bar{V}^{-1}}^2$$
.

The proof can be finished by applying Theorem 1 and Lemma 10 from Abbasi-Yadkori et al. (2011) to bound $||Z||^2_{V^{-1}}$, using $\lambda = 1/2$.

C.4. Proof of Lemma 6

We will prove the first part of the lemma by induction. It is easy to check the lemma holds for s = 1. Suppose we have $a_t^* \in A_s$ and we want to prove $a_t^* \in A_{s+1}$. Since the algorithm proceeds to stage s + 1, we know from step 2b that

$$m_{t,a}^{(s)} - x'_{t,a}\theta^* | \le w_{t,a}^{(s)} \le 2^{-s}$$

for all $a \in A_s$. Specially, it holds for $a = a_t^*$ because $a_t^* \in A_s$ by our induction step. Then the optimality of a_t^* implies

$$m_{t,a_t^*}^{(s)} \ge x_{t,a_t^*}' \theta^* - 2^{-s} \ge x_{t,a}' \theta^* - 2^{-s} \ge m_{t,a}^{(s)} - 2 \cdot 2^{-s}$$

for all $a \in A_s$. Thus we have $a_t^* \in A_{s+1}$ according to step 2d.

Suppose a_t is selected at stage s_t in step 2b. If $s_t = 1$, obviously the lemma holds because $0 \le \mu(x) \le 1$ for all x. If $s_t > 1$, since we have proved $a_t^* \in A_{s_t}$, again step 2b at stage $s_t - 1$ implies

$$|m_{t,a}^{(s_t-1)} - x_{t,a}'\theta^*| \le 2^{-s_t+1}$$

for $a = a_t$ and $a = a_t^*$. Step 2d at stage $s_t - 1$ implies

$$m_{t,a_t^*}^{(s_t-1)} - m_{t,a_t}^{(s_t-1)} \le 2 \cdot 2^{-s_t+1}.$$

Combining above two inequalities, we get

$$x'_{t,a_t}\theta^* \ge m_{t,a_t}^{(s_t-1)} - 2^{-s_t+1} \ge m_{t,a_t^*}^{(s_t-1)} - 3 \cdot 2^{-s_t+1} \ge x'_{t,a_t^*}\theta^* - 4 \cdot 2^{-s_t+1}$$

When a_t is selected in step 2c, since $m_{t,a_t}^{(s_t)} \ge m_{t,a_t}^{(s_t)}$, we have

$$x'_{t,a_t}\theta^* \ge m_{t,a_t}^{(s_t)} - 1/\sqrt{T} \ge m_{t,a_t}^{(s_t)} - 1/\sqrt{T} \ge x'_{t,a_t}\theta^* - 2/\sqrt{T}.$$

Using the fact that $\mu(x_1) - \mu(x_2) \leq L_{\mu}(x_1 - x_2)$ for $x_1 \geq x_2$, we will get the desired result.

C.5. Proof of Lemma 9

Lemma 9. Let a and b be two positive constants. If $m \ge a^2 + 2b$, then $m - a\sqrt{m} - b \ge 0$.

Proof. The function $t \mapsto t^2 - at - b$ is monotonically increasing for $t \ge a/2$. Since $m \ge a^2 + 2b$, we have $\sqrt{m} \ge a/2$, so

$$m - a\sqrt{m} - b \geq a^{2} + 2b - a\sqrt{a^{2} + 2b} - b$$

$$\geq a^{2} + b - a\sqrt{a^{2} + 2b + b^{2}/a^{2}}$$

$$= a^{2} + b - a\sqrt{(a + b/a)^{2}}$$

$$= a^{2} + b - a(a + b/a)$$

$$= 0.$$