Precise Minimax Regret for Logistic Regression

Philippe Jacquet, Gil I. Shamir and Wojciech Szpankowski, *Fellow, IEEE,*

Abstract

We study online logistic regression with binary labels and general feature values in which a learner tries to predict an outcome/ label based on data/ features received in rounds. Our goal is to evaluate precisely the (maximal) *minimax regret* which we analyze using a unique and novel combination of information-theoretic and analytic combinatorics tools such as Fourier transform, saddle point method, and Mellin transform in the multi-dimensional settings.

To be more precise, the pointwise regret of an online algorithm is defined as the (excess) loss it incurs over a constant comparator (weight vector) that is used for prediction. It depends on the feature values, label sequence, and the learning algorithm. In the minimax scenario we seek the best weights for the worst label sequence over a class of label distributions. For dimension $d = o(T^{1/3})$ we show that the maximal minimax regret grows as

$$\frac{d}{2}\log(2T/\pi) + C_d + O(d^{3/2}/\sqrt{T})$$

where T is the number of rounds of running a training algorithm and C_d is explicitly computable constant that depends on dimension d and feature values. For features uniformly distributed on a d-dimensional sphere or ball we estimate precisely the constant C_d showing that $C_d \sim -(d/2)\log(d/\sqrt{2\pi})$ with high probability (whp) leading to the minimax regret growing for large d as $(d/2)\log(T/d) - (d/2)\log(\sqrt{8\pi}) + O(1)$. We also extend these results to non-binary labels. To the best of our knowledge the precise minimax regret presented here is the first result of this kind for a general feature values and wide range of d. This provides a precise answer to the regret evaluation challenge posed in [17].

I. Introduction

In online learning sequentially received data must be used to update the predictor for subsequent data, that is, a model is trained to learn parameters from examples/ samples whose outcomes are already labeled. The training algorithm consumes data in rounds, where at each round $t \in \{1, 2, \ldots, T\}$, it is allowed to predict the label based only on the labels it observed in the past $t-1$ rounds. The prediction algorithm incurs for each round some *loss* and updates its belief of the model parameters. In this paper we study a more specific setting of online *logistic regression* for binary classification. Logistic regression has received a lot of attention in machine learning ([3], [24]) due to several important applications from category classification to risk assessment.

More precisely, we phrase our learning problem in terms of a game between nature/ environment and a learner. At each round the learner obtains a d dimensional input/ feature vector $\mathbf{x}_t$ and makes prediction $\hat{y}_t$. Then the nature reveals the true output/ label y_t. Throughout we assume binary labels $y_t \in \{-1, 1\}$ (however, see Section III-B for extension to non-binary labels) and bounded features $\mathbf{x}_t$ living in a space of dimension d. Thus at round t the learner incurs some *loss* which we denote as $\ell(\hat{y}_t, y_t)$. For $t \in \{1, \ldots, T\}$ we write $y^T = (y_1, \ldots, y_T)$ and $\mathbf{x}^T = (\mathbf{x}_1, \ldots, \mathbf{x}_T)$. Then the cumulative relative loss or better *pointwise regret* is defined as in [11], [9], [28]

$$R_T(\hat{y}^T, y^T|\mathbf{x}^T) = \sum_{t=1}^{T} \ell(\hat{y}_t, y_t) - \inf_{f\in\mathcal{F}} \sum_{t=1}^{T} \ell(f(\mathbf{x}_t), y_t)$$

where $\mathcal{F}$ is a reference class of functions called also forecasters or experts. In this paper, we consider the (maximal) *minimax regret* defined as

$$r_T^*(\mathbf{x}^T) = \inf_{\hat{y}^T} \max_{y^T} R_T(\hat{y}^T, y^T|\mathbf{x}^T) \tag{1}$$

which constitutes a fundamental/ universal lower bound over a class of learning algorithms. This regret could be viewed as "fixed-design" (or conditional) minimax regret with $\mathbf{x}^T$ known in advance. Another minimax regret called here the adversarial minimax regret with known $\mathbf{x}^T$ can be defined as

$$\begin{aligned} r^a(\mathbf{x}^T) &\triangleq \langle\!\langle \min_{\hat{y}_t} \max_{y_t} \rangle\!\rangle_{t=1}^{T} R(\mathbf{x}^T, y^T, \hat{y}^T) \\ &\triangleq \min_{\hat{y}_1} \max_{y_1} \min_{\hat{y}_2} \max_{y_2} \cdots \min_{\hat{y}_T} \max_{y_T} R(\hat{y}^T, y^T|\mathbf{x}^T). \end{aligned} \tag{2}$$

Philippe Jacquet is with INRIA, France, email: philippe.jacquet@inria.fr

Gil I. Shamir is with Giigle, Pitsburgh, PA, USA email: gshamir@ieee.org

W. Szpankowski is with the Department of Computer Science, Purdue University, IN 47907, USA, (e-mail: spa@cs.purdue.edu)

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It was recently proved that $r_T^*(\mathbf{x}^T) = r^a(\mathbf{x}^T)$ [33]. Hereafter, we focus in $r_T(\mathbf{x}^T$ and give precise asymptotic expansion of this regret.

In this paper we consider a more specific model, namely *logistic regression* with logarithmic loss function and linear reference class. More specifically, we restrict the reference class to $\mathcal{F} = \{\mathbf{x}_t \to f(\mathbf{x}_t) = \mathrm{Sigmoid}(\langle \mathbf{x}_t, \mathbf{w}\rangle)\}$ where $\mathrm{Sigmoid}(\langle \mathbf{x}_t, \mathbf{w}\rangle) = (1+\exp(-\langle \mathbf{x}_t, \mathbf{w}\rangle))^{-1}$ is the logistic function and $\langle \mathbf{x}_t, \mathbf{w}\rangle = \sum_{i=1}^d x_{i,t} w_i$ is the scalar product for some weight vector $\mathbf{w} = (w_1, \ldots, w_d)$. We also define

$$\ell(y_t|\mathbf{x}_t, \mathbf{w}) := \ell(f(\mathbf{x}_t), y_t) := \log\left(1+\exp(-y_t\langle \mathbf{x}_t, \mathbf{w}\rangle)\right)$$

as the loss function for the logistic regression.

In the minimax scenario studied in this paper, we postulate that the prediction is based on a learning distribution $Q(y_t|\mathbf{x}_t) = Q(y_t|\hat{y}_t)$ which best approximates the expert prediction $P(y_t|\mathbf{x}_t, \mathbf{w}_t)$. For example, the most popular class of learning algorithms are Bayesian (cf. [9], [15], [28]), but we do *not* make such assumption here. For such a setting the pointwise regret for a *given* learning distribution Q is then defined as

$$R_T(Q, y^T|\mathbf{x}^T) = -\sum_{t=1}^T \log Q(y_t|\mathbf{x}_t) - \inf_{\mathbf{w}} \sum_{t=1}^T \ell(\langle \mathbf{x}_t, \mathbf{w}\rangle, y_t) \tag{3}$$

while the (maximal) minimax regret studied here is

$$r_T^*(\mathbf{x}^T) = \inf_Q \max_{y^T} R_T(Q, y^T|\mathbf{x}^T). \tag{4}$$

Observe that

$$r_T^*(\mathbf{x}^T) \le \max_{y^T} R_T(Q, y^T|\mathbf{x}^T) \tag{5}$$

for any learning algorithm and all label sequences. In this paper we provide a precise asymptotic expansion of the maximal minimax regret, a result that had been wanting for some time.

a) Our Contributions and Methods.: Our contribution is two-fold. First, we present precise asymptotic expansions for the maximal minimax regret (4) through the so called Shtarkov sum (cf. [29], [6]). Second, we apply new methodology using tools of analytic combinatorics such as complex asymptotics and Fourier as well as Mellin transforms (cf [7], [31]) to handle Shtarkov sum for the logistic regression.

More precisely, we first represent the minimax regret (4) as the logarithm of the Shtarkov sum over all label sequences of the optimal label probability which turns out to be the maximum-likelihood distribution as presented in (12). Such a sum arose already in the universal compression as witnessed by [29], [6], [32]. In Theorem 1 we show that for $d = o(T^{1/3})$ the minimax regret grows as

$$\frac{d}{2}\log(2T/\pi) + C_d(\mathbf{x}^T) + O(d^{3/2}/\sqrt{T})$$

where the constant $C_d(\mathbf{x}^T)$ depends on the dimension d and data $\mathbf{x}^T$. We explicitly express this constant as the logarithm of a multi-dimensional integral over the determinant of a matrix that depends on data and the logistic function (cf. (18)). We generalize it to non-binary labels in Theorem 2. Then we find in Theorem 3 an asymptotic expression for $C_d(\mathbf{x}^T)$ when data $\mathbf{x}^T$ are distributed uniformly on a d-dimensional sphere $\mathcal{S}_d$ and a ball $\mathcal{B}_d$. This allows us to show in Theorem 3 that for large d the minimax regret grows with high probability as $\frac{d}{2}\log\frac{T}{d} - \frac{d}{2}\log\sqrt{8\pi} + O(1)$. In Table I we compare our precise findings to known results for the pointwise regret and minimax regret.

Our second technical contribution lies in unique and novel methodology based on analytic combinatorics. As mention above, we represent the maximal minimax regret as a Shtarkov sum. Only recently [25] and [13] introduced Shtarkov sum in the context of logistic regression. To analyze asymptotically the Shtarkov sum, we translate the Shtarkov sum into a d-dimensional integral that we evaluate using a multi-dimensional Laplace/ saddle point method. Further embellishments, including Mellin transform, discrete geometry and spectral representation of matrices, are required to study the constant $C_d(\mathbf{x}^T)$ when the feature $\mathbf{x}^T$ lie on a d-dimensional sphere.

b) Related Work.: In this paper we combine methodology of analytic combinatorics (see, e.g., [7], [14], [31]) and information theory (see, e.g., [1], [6], [16], [19], [22], [23], [26], [35]) to study a machine learning problem (see, e.g., [3], [24]), namely, the regret of logistic regression.

The set up of the logistic regression is similar to the redundancy of universal coding studied extensively in information theory. It corresponds to a single dimensional (i.e., $d = 1$) regret problem for logistic regression. In this case, with m being the alphabet size or the number of labels, it is known that for a large class of sources (up to Markovian but not for non-Markovian as discussed in [4], [8]) the redundancy grows as $\frac{m-1}{2}\log T$ when the alphabet size m is fixed (see [6], [23], [26], [30], [35], [36]) and $\frac{m-1}{2}\log(T/m)$ for $m = o(T)$ (see also [19], [26], [32]). In fact in [32] full asymptotic expansions were derived for all ranges of m.

In the machine learning literature a general online optimization is studied, and generally *pointwise regret* is analyzed with logarithmic regret in the strongly and weakly convex setting. We note that logistic regression seems to fall under weakly convex

TABLE I
COMPARISON OF RESULTS

Problem Setting		Previous Results	This Paper
Binary Labels, $d = 1$	:	$r_T^* = \frac{1}{2}\log T$ [[5]] [[16]] [[18]]	
Multi Labels; $d = 1$ $\omega(1) = m = o(T)$	:	$r_T^* = \frac{m-1}{2}\log(T/m)$ [[16]] [[19]] [[27]]	
Multi Labels; $d = 1$ $m = \alpha T$ $T = o(m)$	:	$\bar{r}_T^* = T\log B_\alpha + O(1)$ [explicit constant B_α] [[32]] $r_T^* = T\log\frac{m}{T} + O(T^2/m)$ [[19], [27], [32]]	
Binary Labels Multi Dimensions d	:	Pointwise regret for Bayesian algorithms Q: $L_2 : \|\mathbf{w}^*\|_2 \leq B$ $O(B\sqrt{dT})$ [[34]] $R_T \leq \frac{d}{2}\log(1+T)$ [[15]] $R_T \leq \frac{d}{2}\log\left(\frac{B^2T}{d} + e\right)$ [[9]] $\frac{d}{2}\log\frac{T}{d^3} \leq R_T \leq \frac{d}{2}\log\frac{B^2T}{d^2}$ [[28]] **Minimax regret**: $\max_{\mathbf{x}^T} r_T^*(\mathbf{x}^T) = O(\text{polylog}(T))$ [[20], [21]] For *finite feature values* and $d = O(1)$: $r_T^* = \frac{d}{2}\log(2T/\pi) + C + O(1/\sqrt{T})$ where C explicit constant [13].	**Minimax regret**: $r_T^*(\mathbf{x}^T) \leq \max_{y^T} R_T(y^T, Q\|\mathbf{x}^T)$, $\forall Q$. For any $\mathbf{x} \in [-1,1]$ and $d = o(T^{1/3})$: $r_T^*(\mathbf{x}^T) = \frac{d}{2}\log(2T/\pi) + C_d(\mathbf{x}^T) + O(d^{3/2}/\sqrt{T})$ where $C_d(\mathbf{x}^T) = \int_{\mathbf{R}^d}\sqrt{\det(\mathbf{B}(\mathbf{w}, \mathbf{x}^T))}d\mathbf{w}$. For $\mathbf{x}_t$ in d-dimensional sphere: $C_d \sim -\frac{d}{2}\log(d/2\pi)$, hence: $r_T^* = \frac{d}{2}\log\frac{T}{d} - \frac{d}{2}\log\sqrt{8\pi} + O(1)$.
Multi Labels m Multi Dimensions d	:	Pointwise regret for Bayesian algorithm: L_2 constraints: $R_T \leq 5md\log\left(\frac{BT}{dm} + e\right)$ [[9]] $\|\mathbf{w}^{*(m)}\|_\infty \leq B$: $R_T \geq \frac{d(m-1)}{2}\log\left(\frac{T}{d\cdot m}\right)$ [[28]] **Minimax regret**: for *finite feature values* for $d, m = O(1)$: $r_T^* = \frac{d(m-1)}{2}\log(2T/\pi) + C_m + O(1/\sqrt{T})$ where C_m explicit constant [13].	**Minimax regret**: $\mathbf{x} \in [-1,1]$ and $md = o(T^{1/3})$: $r_T^* = \frac{d(m-1)}{2}\log(2T/\pi) + C_{m,d} + O((dm)^{3/2}/\sqrt{T})$ where $C_{m,d}$ explicit constant.

setting. We first mention work of [11] who studied the pointwise regret of the logistic regression for the *proper* setting, that is, when at time t the decision regarding $\mathbf{w}_t$ is based on knowledge available to the learner up to time $t-1$. Unlike the *improper* learning, studied in this paper, where feature $\mathbf{x}_t$ at time is also available to the learner and [11] showed that the pointwise regret is $\Theta(T^{1/3})$ for $d = 1$ and $O(\sqrt{T})$ for $d > 1$. Furthermore, the worst case adversarial minimax regret for a wide variety of loss function and references classes is discussed in a series of papers by [20], [21].

For improper learning a more precise results are known. To the best of our knowledge, [15] were first to demonstrate results that suggest that *pointwise regret* for logistic regression grows like $O(d\log T/d)$ where for fixed dimension d and $m = 2$, which was further generalized in [9] to all m. The authors of [15] used *Bayesian model averaging*. The $O(\log T)$ pointwise and individual sequence regret can be achieved for the single dimensional problem with gradient methods based approaches, as was demonstrated in [18]. The authors of [18] then posed the question of what happens for larger dimensions. Subsequently, [9] demonstrated how to achieve regret bounds of $O(d\log(T/d))$ with Bayesian model averaging. These results were strengthened in [28], which also provided matching lower bounds. Recently, [13] analyze a precise maximal minimax regret but only for *finite* number of feature values and fixed dimension d. More precisely, [13] addresses a relaxed problem with at most a finite number $N = o(\sqrt{T})$ of distinct feature vector values and regret is analyzed only for a fixed dimension $d = O(1)$. In this paper we consider: (i) no relaxation, where feature vectors can take any values (up to $N = T$ distinct ones); (ii) the dimension d can grow with T as $d = o(T^{1/3})$; and (iii) a different methodology based on a multidimensional Laplace is used while the analysis of [13] is based on multidimensional Gaussian approximation, which fails in our setting. To the best of our knowledge here we present the first precise results for the minimax regret.

II. Problem Formulation and Notation

We denote by $\mathbf{x}_t = (x_{1,t}, \ldots, x_{d,t})$ a d-dimensional feature vector such that $||x|| \leq 1$ for some norm $||\cdot||$. We also assume that the set $\mathbf{x}_t$ spans $\mathbf{R}^d$. The label binary vector is denoted as $y^T = (y_1, \ldots, y_T)$ with $y_t \in \{-1, 1\}$ (however, we also present in Section III-B some results for non-binary labels). Finally, $\mathbf{w}_t = (w_{1,t}, \ldots, w_{d,t})$ is a d-dimensional vector of weights. In this paper, we do not address the method used to learn the weights (e.g., gradient method or Bayesian mixing), however, see the end of this section for some remarks on a sequential algorithm.

The cumulative *logistic loss* of an algorithm that *plays* $\mathbf{w}_t$ at round t is

$$L(y^T|\mathbf{x}^T, \mathbf{w}^T) := \sum_{t=1}^{T} \log\left[1 + \exp(-y_t\langle \mathbf{x}_t, \mathbf{w}_t\rangle)\right] \tag{6}$$

where $\langle \mathbf{x}_t, \mathbf{w}_t\rangle = \sum_{i=1}^{d} x_{i,t}w_{i,t}$ is the scalar product of $\mathbf{x}_t$ and $\mathbf{w}_t$. To simplify we also write $\ell(y_t|\mathbf{x}_t, \mathbf{w}_t) := \log\left[1 + \exp(-y_t\langle \mathbf{x}_t, \mathbf{w}_t\rangle)\right]$. Both $\ell(y_t|\mathbf{x}_t, \mathbf{w}_t)$ and $L(y^T|\mathbf{x}^T, \mathbf{w}^T)$ depend on $\mathbf{x}_t$ and $\mathbf{w}_t$ only through the product $\langle \mathbf{x}_t, \mathbf{w}_t\rangle$. As mention in the introduction, it is convenient to interpret the logistic function in probabilistic terms. The probability of a label is then given by

$$P(y_t|\mathbf{x}_t, \mathbf{w}_t) = \left(1 + \exp(-y_t\langle \mathbf{x}_t, \mathbf{w}_t\rangle)\right)^{-1} \tag{7}$$

and clearly $\ell(y_t|\mathbf{x}_t, \mathbf{w}_t) = -\log P(y_t|\mathbf{x}_t, \mathbf{w}_t)$.

Finally, we observe that the goal is to find the best learning distribution $Q(y_t|\mathbf{x}_t)$ of the unknown distribution $P(y_t|\mathbf{x}_t, \mathbf{w}_t)$. We notice that Q can be used to design an algorithm that predicts y_t. The *pointwise regret* for a given algorithm/ distribution Q is defined in (3) for individual sequences $(y_t, \mathbf{x}_t)$ following [15], [10], [9], [28]. Thus

$$R_T(Q, y^T|\mathbf{x}^T) = \log \frac{\sup_{\mathbf{w}} P(y^T|\mathbf{x}^T, \mathbf{w})}{Q(y^T|\mathbf{x}^T)} \tag{8}$$

where

$$P(y^T|\mathbf{x}^T, \mathbf{w}) = \prod_{t=1}^{T} \left(1 + \exp(-y_t\langle \mathbf{x}_t, \mathbf{w}\rangle)\right)^{-1}. \tag{9}$$

The pointwise regret $R_T(Q, y^T|\mathbf{x}^T)$ is a function of label sequence y^T, data/ feature vector $\mathbf{x}^T$, and algorithm/ label distribution Q. A better measure of online logistic regression performance should decouple the regret from the fluctuations of y^T (but may still depend on the feature vector $\mathbf{x}^T$) and minimize over a class of learning algorithms/ distributions Q. Following information-theoretic view, as in [5], [6], [36], we define the (maximal) minimax regret (conditioned on $\mathbf{x}^T$) as in (4). Notice that this definition is over all possible learning algorithms represented by Q. Therefore, it constitutes a (universal) lower bound of the pointwise regret – as expressed in (5) – for all label sequences and for all learning distributions Q, including the Bayesian ones studied in [15], [9], [28].

We study in this paper the precise growth of the minimax regret for large T and wide range of d. However, to accomplish it we need a more succinct and computationally manageable representation of the maximal minimax regret. Following [29], [6], [3] we add and subtract from (4) the logarithm of the Shtarkov sum defined as

$$S_T(\mathbf{x}^T) \stackrel{\triangle}{=} \sum_{y^T} \sup_{\mathbf{w}} P(y^T|\mathbf{x}^T, \mathbf{w}) \tag{10}$$

resulting in

$$\begin{aligned} r_T^*(\mathbf{x}^T) &= \min_{Q} \sup_{\mathbf{w}} \max_{y^T} (-\log Q(y^T|\mathbf{x}^T) + \log P^*(y^T|\mathbf{x}^T)) + \log \sum_{y^T} \sup_{\mathbf{w}} P(y^T|\mathbf{x}^T, \mathbf{w}) \\ &= \log \sum_{y^T} \sup_{\mathbf{w}} P(y^T|\mathbf{x}^T, \mathbf{w}) = \log S_T(\mathbf{x}^T) \end{aligned} \tag{11}$$

where we set $Q(y^T, \mathbf{x}^T) = P^*(y^T|\mathbf{x}^T)$ with

$$P^*(y^T|\mathbf{x}^T) := \frac{\sup_{\mathbf{w}} P(y^T|\mathbf{x}^T, \mathbf{w})}{\sum_{v^T} \sup_{\mathbf{w}} P(v^T|\mathbf{x}^T, \mathbf{w})} \tag{12}$$

being the *maximum-likelihood distribution*. Indeed, since Q and P^* are distributions, there is at least one y^T such that the first term in (11) is nonnegative, so that $Q = P^*$ minimizes it (see also [3]). We also observe that the Shtarkov sum is invariant under scaling up data $\mathbf{x}^T$ (and scaling down weights).

Finally, we briefly address the issue of a sequential algorithm. If $\mathbf{x}^T$ as well T are known in advance, we can proceed as follows: Assign conditional probability $Q(y_{t+1}|y^t, \mathbf{x}^{t+1})$ as the quotient of $Q(y^{t+1})/Q(y^t)$ (i.e., the probability of a subsequence up to $t+1$ divided by that of a subsequence up to t). A subsequence probability $Q(y^t)$ is the sum of probabilities on all possible sequences y^T for which y^t is a prefix. Thus all probabilities will be computed directly from the full sequence probabilities of all possible label sequences.

III. Main Results

In this section we estimate asymptotically the Shtarkov sum (10) for large T and wide range of d Throughout we write $p(w) := (1+e^{-w})^{-1}$ and $q(w) = 1-p(w) = p(-w)$.

A. Minimax Regret for General Case

We start with a general expression for the probability $P(y^T|\mathbf{x}^T,\mathbf{w})$ as given in (9). Noting that

$$P(y_t=1|\mathbf{x}_t,\mathbf{w}) = \frac{1}{1+\exp(-\langle \mathbf{x}_t,\mathbf{w}\rangle)} = \frac{\exp(\langle \mathbf{x}_t,\mathbf{w}\rangle)}{1+\exp(\langle \mathbf{x}_t,\mathbf{w}\rangle)}$$

we find

$$P(y^T|\mathbf{x}^T,\mathbf{w}) = \prod_{t=1}^{T} \frac{\exp\left(\frac{1+y_t}{2}\langle \mathbf{x}_t,\mathbf{w}\rangle\right)}{1+\exp(\langle \mathbf{x}_t,\mathbf{w}\rangle)} = \exp\left(-\sum_{t=1}^{T}\log(1+e^{\langle \mathbf{x}_t,\mathbf{w}\rangle}) + \sum_{t=1}^{T}\frac{1+y_t}{2}\langle \mathbf{x}_t,\mathbf{w}\rangle\right).$$

Let now

$$L_T(\mathbf{w}) = L_T(\mathbf{w},\mathbf{x}^T) = \sum_{t=1}^{T}\log(1+e^{\langle \mathbf{w},\mathbf{x}_t\rangle}), \quad \text{and} \qquad \mathbf{A}_T(y^T,\mathbf{x}^T) := \mathbf{A}(y^T) = \frac{1}{2}\sum_{t=1}^{T}(1+y_t)\mathbf{x}_t.$$

Then $P(y^T|\mathbf{x}^T,\mathbf{w})$ becomes

$$P(y^T|\mathbf{x}^T,\mathbf{w}) = \exp\left(-L_T(\mathbf{w},\mathbf{x}^T) + \langle \mathbf{w},\mathbf{A}_T(y^T)\rangle\right). \tag{13}$$

Now we sketch the road map of our approach, leaving technical details to the next section and Appendix. The optimal value $\mathbf{w}^*$ that maximizes $P(y^T|\mathbf{x}^T,\mathbf{w})$ satisfies

$$\nabla_{\mathbf{w}} L_T(\mathbf{w}^*) = \mathbf{A}_T(y^T) \tag{14}$$

where $\nabla L_T(\mathbf{w}^*)$ is the gradient vector of $L_T(\mathbf{w})$. It is easy to see that

$$\mathbf{G}_T(\mathbf{w}) := \nabla_{\mathbf{w}} L_T(\mathbf{w}) = \sum_{t=1}^{T} p(\langle \mathbf{w},\mathbf{x}_t\rangle)\mathbf{x}_t \tag{15}$$

due to the crucial property $p'(w) = p(w)q(w)$. In the next section (see discussion below (32)) we prove that $\mathbf{w}^*$ exists and is unique in $[-\infty,\infty]^d$.

In view of the above, the optimal probability $P^*(y^T|\mathbf{x}^T,\mathbf{w})$ is then

$$P^*(\mathbf{w}^*) = P^*(y^T|\mathbf{x}^T) = \exp(-L_T(\mathbf{w}^*) + \langle \mathbf{w}^*,\mathbf{G}_T(\mathbf{w}^*)\rangle). \tag{16}$$

In the next section, we apply Laplace/Fourier transform to represent the Shtarkov sum $S_T(\mathbf{x}^T)$ as a multidimensional integral that we evaluate using the multidimensional Laplace method. This will allow us to conclude that

$$S_T(\mathbf{x}^T) = \int_{\mathbf{R}^d} \sqrt{\det(\nabla\mathbf{G}(\mathbf{w}^*)/(2\pi)}d\mathbf{w}^* \cdot \left(1+O\left(\frac{d^{3/2}}{\sqrt{T}}\right)\right)$$

where

$$\nabla\mathbf{G}(\mathbf{w}) = \sum_{t=1}^{T} p(\langle \mathbf{w},\mathbf{x}_t\rangle)q(\langle \mathbf{w},\mathbf{x}_t\rangle)\mathbf{x}_t\otimes\mathbf{x}_t.$$

In summary, our first main result proved in the next section can be formulated as follows.

Theorem 1: Let $\mathbf{x}_t \in [-1,1]^d$ and span $\mathbf{R}^d$ as well as $p(w) = (1+e^{-w})^{-1}$ with $q(w) = 1-p(w)$. Then asymptotically for $d = o(T^{1/3})$

$$r^*(\mathbf{x}^T) = \frac{d}{2}\log T - \frac{d}{2}\log 2\pi + C_d(\mathbf{x}^T) + O(d^{3/2}/\sqrt{T}) \tag{17}$$

where the "discrepancy" $C_d(\mathbf{x}^T)$ is

$$C_d(\mathbf{x}^T) = \log\left(\int_{\mathbf{R}^d}\sqrt{\det(\mathbf{B}_d(\mathbf{w},\mathbf{x}^T))}dw_1\cdots dw_d\right) \tag{18}$$

with

$$\mathbf{B}(\mathbf{w},\mathbf{x}^T) = \frac{1}{T}\sum_{t=1}^{T} p(\langle \mathbf{x}_t,\mathbf{w}\rangle)q(\langle \mathbf{x}_t,\mathbf{w}\rangle)\mathbf{x}_t\otimes\mathbf{x}_t \tag{19}$$

and $\mathbf{x}_t\otimes\mathbf{x}_t = \mathbf{x}_t\mathbf{x}_t^\tau$ being the tensor product of $\mathbf{x}_t$ with τ denoting the transpose.

In passing we should observe that if data $\mathbf{X}_t$ is generated by a stationary ergodic source, then by the *ergodic theorem* we conclude that with high probability (whp)

$$\mathbf{B}(\mathbf{w}, \mathbf{X}^T) \to \mathbf{E}_X[\mathbf{B}(\mathbf{w}, \mathbf{X})] \stackrel{\triangle}{=} \bar{\mathbf{B}}(\mathbf{w}) = \mathbf{E}_X[p(\langle \mathbf{X}_1, \mathbf{w}\rangle)\mathbf{X}_1 \otimes \mathbf{X}_1] \tag{20}$$

when $T \to \infty$. Therefore the discrepancy $C_d(\mathbf{x}^T)$ satisfies

$$C_d(\mathbf{X}^T) \to \log\left(\int_{\mathbf{R}^d} \sqrt{\det(\bar{\mathbf{B}}(\mathbf{w})}d\mathbf{w}\right)$$

in probability (see [2]). In the next section we will use this expression to estimate precisely $C_d(\mathbf{x}^T)$ for features $\mathbf{x}^T$ distributed on a sphere and a ball.

B. Extension to Non-binary Labels

Let us now consider a non-binary label alphabet of size m. We will follow [9] and define a matrix $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_{m-1}]$ where each $\mathbf{w}_k$ is a vector of dimension d.The multinomial logistic function known also as *softmax function* is then defined as

$$p_\ell(\mathbf{x}^\tau \mathbf{W}) = \frac{e^{\langle \mathbf{x}, \mathbf{w}_\ell\rangle}}{1 + \sum_{k=1}^{m-1} e^{\langle \mathbf{x}, \mathbf{w}_k\rangle}} \qquad \text{and} \qquad q(\mathbf{x}^\tau \mathbf{W}) = 1 - \sum_{\ell=1}^{m-1} p_\ell(\mathbf{x}^\tau \mathbf{W}) \tag{21}$$

for $\ell = 1, \ldots, m-1$. Alternatively, we can express $\langle \mathbf{x}, \mathbf{w}_\ell\rangle$ as $\langle \mathbf{x}, \mathbf{W}\mathbf{e}_\ell\rangle$ where $\mathbf{e}_\ell$ is a column vector of dimension $m-1$ with all coefficient equal to zero except the ℓth coefficient which is set at 1. We also have $\langle \mathbf{x}, \mathbf{w}_\ell\rangle = \mathrm{tr}(\mathbf{W}\mathbf{e}_\ell \otimes \mathbf{x}^\tau)$. Finally, we write $\mathbf{p} = (p_1, \ldots, p_m)$.

Following the footsteps of our derivations for the binary labels, in Appendix 0a we present a brief proof of our next result.

Theorem 2: Let $\mathbf{x}_t \in [-1, 1]^d$ and span $\mathbf{R}^d$. The label alphabet is of size m, and for $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_{m-1}]$ we define $p_\ell(\mathbf{x}^\tau \mathbf{W})$ for $\ell = 1, \ldots, m-1$ as in (21). Then asymptotically for $md = o(T^{1/3})$

$$r^*(\mathbf{x}^T) = \frac{d(m-1)}{2}\log\frac{T}{2\pi} + \log\left(\int_{\mathbf{R}^{d(m-1)}} \sqrt{\det(\mathbf{B}(\mathbf{W}))}d\mathbf{w}_1 \cdots d\mathbf{w}_{m-1}\right) + O((md)^{3/2}/\sqrt{T}) \tag{22}$$

where

$$\mathbf{B}(\mathbf{W}) = \frac{1}{T}\sum_{t=1}^{T} \mathbf{x}_t \otimes [\mathrm{Diag}\,(\mathbf{p}(\mathbf{x}_i^\tau \mathbf{W})) - \mathbf{p}(\mathbf{x}_i^\tau \mathbf{W}) \otimes \mathbf{p}(\mathbf{x}_i^\tau \mathbf{W})] \otimes \mathbf{x}_t.$$

is a $d(m-1) \times (m-1)d$ matrix.

C. Spherical Features

Now we assume that the feature $\mathbf{x}_t$ are either uniformly distributed on a d-dimensional sphere $\mathcal{S}_d$ or inside a d-dimensional ball $\mathcal{B}_d$ for large d. We explain our ideas on $\mathbf{x}_t$ distributed uniformly on the sphere $\mathcal{S}_d$ of radius 1. By (20) we know that with high probability (whp)

$$\mathbf{B}(\mathbf{w}, \mathcal{S}_d) \to \bar{\mathbf{B}}(\mathbf{w}) = \frac{1}{s_d}\int_{\mathcal{S}_d} p(\langle \mathbf{x}\mathbf{w}\rangle)q(\langle \mathbf{x}\mathbf{w}\rangle)\mathbf{x} \otimes \mathbf{x}\; d\mathbf{x} \tag{23}$$

where s_d is the area of the hypersphere of dimension d and radius 1, that is, $s_d = 2\pi^{(d+1)/2}/\Gamma(\frac{d+1}{2})$.

We first present the following lemma that we prove in the Appendix A using analytic tools such as complex asymptotics and Mellin transform as discussed in [31].

Lemma 1: Let $f(x) = p(x)q(x) = [(1+e^{-x})(1+e^x)]^{-1}$ and $\mathbf{u} = \mathbf{w}/||\mathbf{w}||$.
(i) We have the following expression

$$\bar{\mathbf{B}}(\mathbf{w}) = \mu(\mathbf{w})(\mathbf{I}_d - \mathbf{u} \otimes \mathbf{u}) + \lambda(\mathbf{w})\mathbf{u} \otimes \mathbf{u} \tag{24}$$

where $\mathbf{I}_d$ is the identity operator on $\mathbf{R}^d$ (thus $\mathbf{I}_d - \mathbf{u} \otimes \mathbf{u}$ is the identity operator on the hyperplane orthogonal to $\mathbf{u}$) and

$$\lambda(\mathbf{w}) = \frac{s_{d-1}}{s_d}\int_0^\pi \cos(\theta)^2 \sin(\theta)^{d-2} f(\cos(\theta)\|\mathbf{w}\|)d\theta, \quad \mu(\mathbf{w}) = \frac{s_{d-1}}{s_d}\int_0^\pi \frac{\sin(\theta)^d}{d-1} f(\cos(\theta)\|\mathbf{w}\|)d\theta \tag{25}$$

are the eigenvalues of $\bar{\mathbf{B}}(w)$ with multiplicity 1 and $d-1$, respectively.

(ii) Furthermore, $\det\bar{\mathbf{B}}(w) = \lambda(\mathbf{w}) \cdot \mu^{d-1}(\mathbf{w})$ and both $\lambda(\mathbf{w})$ and $\mu(\mathbf{w})$ are of order $O(\|\mathbf{w}\|^{-3})$ so that $\det(\bar{\mathbf{B}}(\mathbf{w}))$ is $O(\|\mathbf{w}\|^{-3d})$. More precisely,

$$\det(\bar{\mathbf{B}}(\mathbf{w})) = 2\left(\frac{s_{d-1}}{3s_d}\pi^2\|\mathbf{w}\|^{-3}(1 + O(\|\mathbf{w}\|^{-2}))\right)^d \tag{26}$$

for large $\|\mathbf{w}\| \to \infty$.

We now write $C_d(\mathcal{S}_d)$ and $C_d(\mathcal{B}_d)$ for $C_d(\mathbf{x}^T)$ when $\mathbf{x}^T$ lies on the sphere $\mathcal{S}_d$ and on the ball $\mathcal{B}_d$, respectively. Using Lemma 1 we prove in the next section the following theorem.

Theorem 3: Under assumptions of Theorem 1 let us now postulate that the feature vector lies on the d-dimensional sphere $\mathcal{S}_d$ or ball $\mathcal{B}_d$. Then with high probability

$$C_d(\mathcal{S}_d) = -\frac{d}{2}\log\frac{d}{4} + \frac{d}{4}\log(\pi/8) + \frac{3}{8}\log e + O(1/d) \tag{27}$$

and

$$C_d(\mathcal{B}_d) = -\frac{d}{2}\log\frac{d}{4} + \frac{d}{4}\log(\pi/8) - \frac{1}{8}\log e + O(1/d), \tag{28}$$

respectively. Furthermore, the minimax regret $r_T^*(\mathcal{S}_d)$ for features lying uniformly on the sphere $\mathcal{S}_d$ converges with high probability to

$$r_T^*(\mathcal{S}_d) = \frac{d}{2}\log\frac{T}{d} - \frac{d}{2}\log\sqrt{8\pi} + \frac{3}{8}\log e + O(d^{3/2}/\sqrt{T})$$

and for the features inside a d dimensional ball $\mathcal{B}_d$ we find

$$r_T^*(\mathcal{B}_d) = \frac{d}{2}\log\frac{T}{d} - \frac{d}{2}\log\sqrt{8\pi} - \frac{1}{8}\log e + O(d^{3/2}/\sqrt{T})$$

for large d.

Remark 1: In passing we remark that our results and [28] allow us to provide the first order asymptotics for the adversarial maximal minimax regret defined as [20]

$$r_T^a \stackrel{\triangle}{=} \langle\!\langle \max_{\mathbf{x}_t} \min_{\hat{y}_t} \max_{y_t} \rangle\!\rangle_{t=1}^T R(\mathbf{x}^T, y^T, \hat{y}^T).$$

By max-min inequality we first conclude that $r_T^a \geq \max_{\mathbf{x}^T} r_T^*(\mathbf{x}^T)$. Using the upper bound of [28] and our Theorem 1 we easily find (see also [33])

$$r_T^a \sim \frac{d}{2}\log T$$

for large T and $d = o(T^{1/3})$. This seems to be the first precise asymptotics for the adversarial minimax regret with logarithmic loss.

IV. Analysis

A. Proof of Theorem 1

Let $\mathcal{A}_T(\mathbf{x}^T)$ be the set of achievable partial sums of the vectors $\mathbf{x}_t$, i.e.,

$$\mathcal{A}_T := \mathcal{A}_T(\mathbf{x}^T) = \{\mathbf{a} \in \mathbf{R}^d : \ \exists y^T \in \{-1,1\}^T : \ \mathbf{A}_T(y^T) = \mathbf{a}\}$$

and let $N(\mathbf{A})$ be the number of y^T tuples such that $\mathbf{A}_T(y^T) = \mathbf{A}$. The enumeration Laplace-like function of $e^{\langle \mathbf{w}, \mathbf{A}\rangle}$ then satisfies

$$F_T(\mathbf{w}) = \sum_{y^T} e^{\langle \mathbf{w}, \mathbf{A}\rangle} = \prod_t (1 + e^{\langle \mathbf{w}, \mathbf{x}_t\rangle}) = \exp(L_T(\mathbf{w})) \tag{29}$$

which can also be written as

$$F_T(\mathbf{w}) = \int e^{\langle \mathbf{w}, \mathbf{A}\rangle} d\rho_T(\mathbf{A}) \qquad \text{with} \qquad \rho_T = \sum_{\mathbf{a}\in\mathcal{A}_T} N(\mathbf{a})\delta_{\mathbf{a}} \tag{30}$$

where $\delta_{\mathbf{a}}$ is the Dirac function on vector $\mathbf{a}$ and ρ_T is viewed as a measure. Using (16) and above we can re-write the Shtarkov sum as

$$S_T(\mathbf{x}^T) = \sum_{\mathbf{A}\in\mathcal{A}_T(\mathbf{x}^T)} N_T(\mathbf{A}) \exp(-L(\mathbf{w}^*(\mathbf{A})) + \langle \mathbf{w}^*(\mathbf{A}), \mathbf{A}\rangle) \tag{31}$$

that we evaluate asymptotically for large T.

We now express (31) as

$$S_T(\mathbf{x}^T) = \int K(\mathbf{A}) d\rho_T(\mathbf{A}), \qquad \text{where} \qquad K(\mathbf{A}) = \exp(-L(\mathbf{w}^*(\mathbf{A})) + \langle \mathbf{w}^*(\mathbf{A}), \mathbf{A}\rangle). \tag{32}$$

Here $\mathbf{w}^*(\mathbf{A})$ is the inverse of function $\mathbf{G}_T(\mathbf{w})$. This inverse exists because the function $L(\mathbf{w})$ is in C^∞ and it is convex since its second derivative $\nabla^2 L(\mathbf{w}) = \sum_t p(\langle \mathbf{x}_t p(\mathbf{w})\rangle) q(\langle \mathbf{x}_t p(\mathbf{w})\rangle) \mathbf{x}_t \otimes \mathbf{x}_t$ is strictly positive as soon as $\mathbf{R}^d$ is spanned by $\mathbf{x}_t$. Therefore, it has a unique minimum although it can have some infinite coordinates. In some cases the minimum can be at infinity. Indeed, consider the case when the pairs $(\mathbf{x}_t, y_t)$ form a separable set, *i.e* for binary labels there is an hyperplane that separates the +1 labelled features from the -1 labelled features. In this case let $\mathbf{w}_0$ be such that $\langle \mathbf{w}_0, \mathbf{x}_t\rangle > 0$ for all $y_t = 1$ and

$\langle \mathbf{w}_0, \mathbf{x}_t \rangle < 0$ otherwise. The minimum is reached at $\mathbf{w}_0 = +\infty$ since $\lim \nabla L(\mathbf{w}) = \mathbf{A}$ when $\mathbf{w} = x\mathbf{w}_0$ with $x \to +\infty$. There can be hybrid cases where the minimum is attained over $\pm\infty$ for some coordinates of $\mathbf{w}$ while the other components remain finite. The example is when the pair label features are separable on some components but are not on the other components. We conclude that $K(\mathbf{A})$ is in C^∞ and has a finite support contained in $[-T, T]^d$.

Let now

$$K^*(\mathbf{w}) = \int_{\mathbf{R}^d} K(\mathbf{A}) e^{i\langle \mathbf{w}, \mathbf{A} \rangle} d\mathbf{A}$$

be the Fourier transform of function $K(\mathbf{A})$. Parseval theorem for multidimensional Fourier transform tells us that

$$S_T(\mathbf{x}^T) = \frac{1}{(2\pi)^d} \int_{\mathbf{c}+\mathbf{R}^d} F_T(i\mathbf{w}) K^*(-\mathbf{w}) d\mathbf{w} \tag{33}$$

where $\mathbf{c}$ is any constant in the domain of the Fourier existence. Notice that

$$K^*(\mathbf{w}) = \int_{\mathbf{R}^d} \exp(-L_T(\mathbf{w}^*(\mathbf{A})) + \langle (\mathbf{w}^*(\mathbf{A}) + i\mathbf{w}), \mathbf{A} \rangle) d\mathbf{A}.$$

By change of variable $\mathbf{A} = \mathbf{G}(\mathbf{w}^*)$ we arrive at

$$K^*(\mathbf{w}) = \int_{\mathbf{R}^d} \exp(-L_T(\mathbf{w}^*) + \langle (\mathbf{w}^* + i\mathbf{w}), \mathbf{G}(\mathbf{w}^*) \rangle) \det(\nabla \mathbf{G}(\mathbf{w}^*)) d\mathbf{w}^* \tag{34}$$

leading to

$$\begin{aligned} S_T(\mathbf{x}^T) &= \frac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \exp(-L_T(\mathbf{w}^*) + \langle \mathbf{w}^*, \mathbf{G}_T(\mathbf{w}^*) \rangle) \det(\nabla \mathbf{G}_T(\mathbf{w}^*)) d\mathbf{w}^* \\ &\cdot \int_{-i\mathbf{c}+\mathbf{R}^d} \exp(L_T(i\mathbf{w}) - i\langle \mathbf{w}, \mathbf{G}_T(\mathbf{w}^*) \rangle) d\mathbf{w}. \end{aligned} \tag{35}$$

We now take the advantage of the fact that the functions under the integrals are analytic functions so that we can move the path of integration of the second integral from $-i\mathbf{c} + \mathbf{R}^d$ to $-i\mathbf{w}^* + \mathbf{R}^d$, finding

$$\begin{aligned} S_T(\mathbf{x}^T) &= \frac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \exp(-L_T(\mathbf{w}^*) + \langle \mathbf{w}^*, \mathbf{G}_T(\mathbf{w}^*) \rangle) \det(\nabla \mathbf{G}_T(\mathbf{w}^*)) d\mathbf{w}^* \\ &\cdot \int_{-i\mathbf{w}^*+\mathbf{R}^d} \exp(L_T(i\mathbf{w}) - i\langle \mathbf{w}, \mathbf{G}_T(\mathbf{w}^*) \rangle) d\mathbf{w}. \end{aligned} \tag{36}$$

Finally, we notice that on the segment $\Im(\mathbf{w}) = i\mathbf{w}^*$ the quantity $|L_T(i\mathbf{w}) - i\langle \mathbf{w}, \mathbf{G}_T(\mathbf{w}^*) \rangle|$ attains its maximum at $\mathbf{w} = -i\mathbf{w}^*$, since

$$\nabla(L_T(i\mathbf{w}) - i\langle \mathbf{w}, \mathbf{G}_T(\mathbf{w}^*) \rangle) = i\mathbf{G}_T(i\mathbf{w}) - i\mathbf{G}_T(\mathbf{w}^*)$$

is zero when $i\mathbf{w} = \mathbf{w}^*$. Hence, for $\mathbf{x} \to 0$ we conclude

$$\begin{aligned} L_T(\mathbf{w}^* + i\mathbf{x}) - \langle (\mathbf{w} + i\mathbf{x}), \mathbf{G}_T(\mathbf{w}^*) \rangle &= L_T(\mathbf{w}^*) - \langle (\mathbf{w}, \mathbf{G}_T(\mathbf{w}^*) \rangle \\ &\quad -\frac{1}{2} \langle \mathbf{x}, \nabla^2, L_T(\mathbf{w}^*) \mathbf{x} \rangle + O(L_T^{(3)}(\mathbf{w}^*) \|\mathbf{x}\|^3) \end{aligned}$$

where $L_T^{(3)}(\mathbf{w}^*)$ is the third derivative of $L_T(\mathbf{w})$ at $\mathbf{w}^*$. But $\nabla^2 L_T(\mathbf{w})$ and $L_T^{(3)}(\mathbf{w}^*)$ are of order $O(T)$, hence we can apply the multidimensional Laplace method to find

$$\int_{\Im(\mathbf{w})=i\mathbf{w}^*} \exp\left(L_T(\mathbf{w}) - \langle \mathbf{w}, \mathbf{G}_T(\mathbf{w}^*) \rangle\right) d\mathbf{w} = \frac{\exp(L_T(\mathbf{w}^*) - \langle \mathbf{w}^*, \mathbf{G}_T(\mathbf{w}^*) \rangle)}{\sqrt{\det(\nabla^2 L_T(\mathbf{w}^*)/(2\pi))}} \tag{37}$$

$$\times \left(1 + O\left(\frac{d^{3/2}}{\sqrt{T}}\right)\right). \tag{38}$$

Since $\exp(L_T(\mathbf{w}^*) - \langle \mathbf{w}^*, \mathbf{G}_T(\mathbf{w}^*) \rangle)$ cancels factor $\exp(-L_T(\mathbf{w}^*) + \langle \mathbf{w}^*, \mathbf{G}_T(\mathbf{w}^*) \rangle)$ in (36) we find the leading expression for $S_T(\mathbf{x}^T)$. The error term follows from [12] using

$$\int_{\mathbf{R}^d} |x|^3 \exp(-a|x|^2) = 1/a^{(d+3)/2} \pi^{d/2} \frac{\Gamma(d/2 + 3/2)}{\Gamma(d/2)} \tag{39}$$

and applying the Stirling formula to the gamma function for large d. After substituting it in (36), we complete the proof of Theorem 1. Details are discussed in Appendix 0a.

B. Proof of Theorem 3

In order to prove asymptotic results of Theorem 3, we must evaluate the quantities $\lambda(\mathbf{w})$ and $\mu(\mathbf{w})$, the eigenvalues of matrix $\bar{\mathbf{B}}(\mathbf{w})$ for large d. The main contribution of both integrals is for θ around $\frac{\pi}{2}$. For $\theta = \frac{\pi}{2} + \sqrt{\frac{2}{d}}x$ we have

$$\left\{\begin{array}{rcl} \sin(\theta)^{d-2} & = & \exp(-\frac{d-2}{d}(x^2+O(x^4))), \\ \cos(\theta)^2 & = & \frac{2}{d}x^2 - 4/(3d^2)x^4 + O(x^6/d^3), \\ f(\cos(\theta)\|\mathbf{w}\|) & = & \frac{1}{4}\exp\left(-\frac{\|\mathbf{w}\|^2}{2d}x^2\right)\cdot(1+O(w^4x^4/d^2) \end{array}\right. \tag{40}$$

leading to (after dropping the error term which is easy to estimate)

$$\begin{aligned} \int_0^\pi \sin(\theta)^{d-2}\cos(\theta)^2 f(\cos(\theta)\|\mathbf{w}\|)d\theta &= (2/d)^{3/2}\int_{-\infty}^{+\infty}\exp\left(-(1+\frac{\|\mathbf{w}\|^2-4}{2d})x^2\right)x^2dx \\ &= (2/d)^{3/2}\frac{\sqrt{\pi}}{2}\left(1+\frac{\|\mathbf{w}\|^2-4}{2d}\right)^{-3/2} \end{aligned} \tag{41}$$

and

$$\begin{aligned} \int_0^\pi \sin(\theta)^{d} f(\cos(\theta)\|\mathbf{w}\|)d\theta &= (2/d)^{1/2}\int_{-\infty}^{+\infty}\exp\left(-(1+\frac{\|\mathbf{w}\|^2}{2d})x^2\right)dx \\ &= (2/d)^{1/2}\sqrt{\pi}\left(1+\frac{\|\mathbf{w}\|^2}{2d}\right)^{-1/2}. \end{aligned} \tag{42}$$

In summary

$$\det(\mathbf{B}(\mathbf{w})) = \left(\frac{s_{d-1}}{s_d}\right)^d (2/d)^{d/2}\frac{1}{d}\frac{1}{(d-1)^{d-1}}\pi^{d/2}\exp\left(-\frac{\|\mathbf{w}\|^2}{4}\right). \tag{43}$$

To complete the derivation, we need to integrate $\sqrt{\det(\mathbf{B}(\mathbf{w}))}$ over the vectors $\mathbf{w}$. This leads to

$$\int\sqrt{(\det(\mathbf{B}(\mathbf{w}))}d\mathbf{w} = \frac{1}{2^d}\left(\frac{s_{d-1}}{s_d}\right)^{d/2}(2/d)^{d/4}\frac{1}{\sqrt{d}}\frac{1}{\sqrt{d-1}^{d-1}}\pi^{d/4}(2\sqrt{2\pi})^d. \tag{44}$$

The final touch is to get an estimate of the ratio $\frac{s_{d-1}}{s_d}$. But

$$\frac{s_{d-1}}{s_d} = \sqrt{\pi}\frac{\Gamma(d/2)}{\Gamma((d-1)/2)}, \qquad \frac{\Gamma(d/2)}{\Gamma(d-1)} = \sqrt{\frac{d}{2}-\frac{1}{4}+O(1/d)}$$

so that

$$\int\sqrt{(\det(\mathbf{B}(\mathbf{w}))}d\mathbf{w} = (\pi/8)^{d/4}e^{3/8}(d/4)^{-d/2} \tag{45}$$

which completes the derivation of (27).

We prove (28) in a similar manner where the extra factor $\left(\frac{d}{d-1}\right)^{d/2}\left(\frac{d-1}{d+1}\right)^{\frac{d-1}{2}}$ comes from the volume of a ball. At the end, for the unit ball features we find

$$\int\sqrt{\det(\mathbf{B}(\mathbf{w}))}d\mathbf{w} = (\pi/8)^{d/4}e^{-1/8}(d/4)^{-d/2}. \tag{46}$$

More details can be found in the Appendix A.

APPENDIX

We prove here Lemma 1 that we repeat below for the reader convenience.

Lemma 2: Let $f(x) = p(x)q(x) = [(1+e^{-x})(1+e^x)]^{-1}$ and $\mathbf{u} = \mathbf{w}/||\mathbf{w}||$.

(i) We have the following expression

$$\bar{\mathbf{B}}(\mathbf{w}) = \mu(\mathbf{w})(\mathbf{I}_d - \mathbf{u}\otimes\mathbf{u}) + \lambda(\mathbf{w})\mathbf{u}\otimes\mathbf{u} \tag{47}$$

where $\mathbf{I}_d$ is the identity operator orthogonal to $\mathbf{u}$ and

$$\lambda(\mathbf{w}) = \frac{s_{d-1}}{s_d}\int_0^\pi \cos(\theta)^2\sin(\theta)^{d-2}f(\cos(\theta)\|\mathbf{w}\|)d\theta \tag{48}$$

and

$$\mu(\mathbf{w}) = \frac{s_{d-1}}{s_d}\int_0^\pi \frac{\sin(\theta)^d}{d-1}f(\cos(\theta)\|\mathbf{w}\|)d\theta \tag{49}$$

are the eigenvalues of $\bar{\mathbf{B}}(w)$ with cardinality 1 and $d-1$, respectively.

(ii) Furthermore, $\det\bar{\mathbf{B}}(w) = \lambda(\mathbf{w})\cdot\mu^{d-1}(\mathbf{w})$ and both $\lambda(\mathbf{w})$ and $\mu(\mathbf{w})$ are of order $O(\|\mathbf{w}\|^{-3})$ and $\det(\mathbf{B}(\mathbf{w}))$ is $O(\|\mathbf{w}\|^{-3d})$. More precisely,

$$\det(\mathbf{B}(\mathbf{w}^*)) = 2\left(\frac{s_{d-1}}{3s_d}\pi^2\|\mathbf{w}\|^{-3}(1+O(\|\mathbf{w}\|^{-2}))\right)^d \tag{50}$$

for large $\|\mathbf{w}\|\to\infty$.

We start with part (i). Let θ be the angle between $\mathbf{x}$ and $\mathbf{u}$. We have the decomposition $\mathbf{x} = \cos(\theta)\mathbf{u}+\mathbf{b}$ with $\mathbf{b}\in\sin\theta\mathcal{S}_{d-1}(\mathbf{u})$ where $\mathcal{S}_{d-1}(\mathbf{u})$ is the unit hypersphere orthogonal to $\mathbf{u}$. Since $\mathbf{x}$'s have a spheric symmetry in its distribution, so it is the case for the $\mathbf{b}$'s in $\sin\theta\mathcal{S}_{d-1}(\mathbf{u})$ for any given angle θ. Thus

$$\begin{aligned}\bar{\mathbf{B}}(\mathbf{w}) &= \frac{1}{s_d}\int_0^\pi f(\|\mathbf{w}\|\cos\theta)d\theta\int_{\sin\theta\mathcal{S}_{d-1}(\mathbf{u})}(\mathbf{b}+\cos\theta\mathbf{u})\otimes(\mathbf{b}+\cos\theta\mathbf{u})d\mathbf{b} &(51)\\ &= \frac{1}{s_d}\int_0^\pi f(\|\mathbf{w}\|\cos\theta)d\theta\int_{\sin\theta\mathcal{S}_{d-1}(\mathbf{u})}(\mathbf{b}\otimes\mathbf{b}+(\cos\theta)^2\mathbf{u}\otimes\mathbf{u})d\mathbf{b}\\ &\quad+\frac{1}{s_d}\int_0^\pi f(\|\mathbf{w}\|\cos\theta)d\theta\int_{\sin\theta\mathcal{S}_{d-1}(\mathbf{u})}\cos\theta(\mathbf{b}\otimes\mathbf{u}+\mathbf{u}\otimes\mathbf{b})d\mathbf{b}. &(52)\end{aligned}$$

Again due to the spheric symmetry of $\mathbf{b}$ we also have $\int_{\sin\theta\mathcal{S}_{d-1}(\mathbf{u})}\mathbf{b}=0$ leading to

$$\begin{aligned}\bar{\mathbf{B}}(\mathbf{w}) &= \frac{1}{s_d}\int_0^\pi f(\|\mathbf{w}\|\cos\theta)d\theta\int_{\sin\theta\mathcal{S}_{d-1}(\mathbf{u})}(\mathbf{b}\otimes\mathbf{b}+(\cos\theta)^2\mathbf{u}\otimes\mathbf{u}d\mathbf{b}\\ &= \frac{1}{s_d}\int_0^\pi f(\|\mathbf{w}\|\cos\theta)(\sin\theta)^{d-1}d\theta\\ &\quad\int_{\mathcal{S}_{d-1}(\mathbf{u})}((\sin\theta)^2\mathbf{b}\otimes\mathbf{b}+(\cos\theta)^2\mathbf{u}\otimes\mathbf{u})d\mathbf{b}. &(53)\end{aligned}$$

The $(\sin\theta)^{d-1}$ factor arises from the change of integration domain from $\sin\theta\mathcal{S}_{d-1}(\mathbf{u})$ to $\mathcal{S}_{d-1}(\mathbf{u})$.

The quantity $\int_{\mathcal{S}_{d-1}(\mathbf{u})}\mathbf{b}\otimes\mathbf{b}$ is the $(d-1)\times(d-1)$ matrix whose (i,j) coefficient is $\int_{\mathcal{S}_{d-1}}b_ib_jd\mathbf{b}$. Clearly, by spheric symmetry of the $\mathbf{b}$ vectors $\int_{\mathcal{S}_{d-1}}b_ib_jd\mathbf{b}=0$ when $i\neq j$. We also have for all $i\neq j$:

$$\int_{\mathcal{S}_{d-1}}(b_i)^2d\mathbf{b} = \int_{\mathcal{S}_{d-1}}(b_j)^2d\mathbf{b} = \frac{1}{d-1}\int_{\mathcal{S}_{d-1}}\|\mathbf{b}\|^2d\mathbf{b} = \frac{s_{d-1}}{d-1}. \tag{54}$$

Thus

$$\int_{\mathcal{S}_{d-1}(\mathbf{u})}\mathbf{b}\otimes\mathbf{b}d\mathbf{b} = \frac{s_{d-1}}{d-1}\mathbf{I}_{d-1}(\mathbf{u}) \tag{55}$$

and similarly

$$\int_{\mathcal{S}_{d-1}(\mathbf{u})}\mathbf{u}\otimes\mathbf{u}d\mathbf{b} = s_{d-1}\mathbf{u}\otimes\mathbf{u} \tag{56}$$

which completes the proof of part (i) of the lemma.

Now we move to part (ii) of Lemma 1. Both $\lambda(\mathbf{w})$ and $\mu(\mathbf{w})$ are functions of $w=\|\mathbf{w}\|$. We write $\lambda(w)=\lambda(\|\mathbf{w}\|)$ and $\mu(w)=\mu(\|\mathbf{w}\|)$. To capture the asymptotics of these functions we apply Mellin transform which is an effective tool of analytic combinatorics for complex asymptotics. The reader is refereed to [7] and [31] for detailed discussions.

The Mellin transforms $\lambda^*(s)$ and $\mu^*(s)$ of $\lambda(w)$ and $\mu(w)$ are defined, respectively, as

$$\begin{aligned}\lambda^*(s) &= \int_0^\infty\lambda(w)w^{s-1}dw,\\ \mu^*(s) &= \int_0^\infty\mu(w)w^{s-1}dw.\end{aligned}$$

Observe now that

$$\begin{aligned}\lambda(w) &= 2\frac{s_{d-1}}{s_d}\int_0^{\pi/2}f(\cos(\theta)w)\cos^2(\theta)\sin^{d-2}(\theta)d\theta &(57)\\ &= \frac{2s_{d-1}}{s_d}\int_0^1 y^2(1-y^2)^{(d-3)/2}f(yx)dy &(58)\end{aligned}$$

via the change of variable $y = \cos(\theta)$. Thus we find

$$\begin{aligned}\lambda^*(s) &= \frac{2s_{d-1}}{s_d}\int_0^1 (1-y^2)^{(d-3)/2}y^2dy\int_0^\infty f(yx)x^{s-1}dx &(59)\\ &= \frac{2s_{d-1}}{s_d}f^*(s)\int_0^1(1-y^2)^{(d-3)/2}y^{2-s}dy &(60)\\ &= f^*(s)\beta_1^*(3-s) &(61)\end{aligned}$$

where $f^*(s)$ is the Mellin transform of $f(x) = p(x)q(x)$ and $\beta_1(s)$ is the Mellin transform of the function $(1-y^2)^{(d-3)/2}y$ defined over $[0,1]$.

The Mellin transform $\beta_1^*(s)$ is defined for $\Re(s) > 0$ and being locally analytical it has poles on the negative even integers, corresponding to the Taylor expansion of $(1-y^2)^{(d-3)/2}$. The Mellin transform $f^*(s)$ of function $f(x)$ is

$$f^*(s) = (s-1)^2(s-2)h^*(s-2)$$

where $h^*(s)$ is the Mellin transform of function $h(x) = \log(1+e^{-x})$ defined for $\Re(s) > 0$. The Mellin transform $f^*(s)$ is defined for $\Re(s > 2$ but the simple poles at $s = 1$ and $s = 2$ are canceled by the factor $(s-1)(s-2)$ thus is finally defined for $\Re(s) > 0$. More precisely, we have

$$h^*(s) = (1-2^{-s})\zeta(s+1)\Gamma(s)$$

where $\Gamma(s)$ is the Euler gamma function and $\zeta(s)$ is the Riemann zeta function.

The product $\beta(2-s)(s-1)^2(s-2)h^*(s-2)$ is defined for $\Re(s) \in [0,1]$. But the simple pole at $s = 1$ is canceled by the additional factor $(s-1)$. The next pole is at $s = 3$ which has the residue $-\zeta(2)\Gamma(3) = -\pi^2/3$, thus $\lambda^*(s)$ is defined for $\Re(s) \in]0,3[$.

We can make a similar analysis for $\mu^*(s)$ and we arrive at

$$\begin{aligned}\lambda^*(s) &= 2\frac{s_{d-1}}{s_d}\beta_1^*(3-s)f^*(s),\\ \mu^*(s) &= 2\frac{s_{d-1}}{(d-1)s_d}\beta_2^*(1-s)f^*(s),\end{aligned}$$

where $\beta_1^*(s)$ and $\beta_2^*(s)$ are respectively the Mellin transform of function $(1-y^2)^{(d-3)/2}$ and function $(1-y^2)^{(d-1)/2}$. The Mellin transform $\mu^*(s)$ is also defined on $\Re(s) \in]0,3[$ and has a simple pole at $s = 3$ with residue $-\zeta(2)\Gamma(3)\frac{d-1}{2} = -\pi^2/6(d-1)$. For both $\lambda^*(s)$ and $\mu^*(s)$ the next pole is at $s = 5$.

We now apply the inverse Mellin transform defined as (e.g., see [31])

$$\begin{aligned}\lambda(w) &= \textstyle\int_{\Re(s)=1}\lambda^*(s)w^{-s}ds,\\ \mu(w) &= \textstyle\int_{\Re(s)=1}\mu^*(s)w^{-s}ds\end{aligned} \quad (62)$$

to extract asymptotics of $\lambda(w)$ and $\mu(w)$ for $w \to \infty$. By moving the integration path over the simple poles at $s = 3$ and $s = 5$ and catching the residues we finally obtain

$$\begin{aligned}\lambda(w) &= 2\tfrac{s_{d-1}}{3s_d}\pi^2w^{-3} + O(w^{-5}),\\ \mu(w) &= \tfrac{s_{d-1}}{3s_d}\pi^2w^{-3} + O(w^{-5})\end{aligned} \quad (63)$$

for $w \to \infty$. In conclusion

$$\det(\bar{\mathbf{B}}(\mathbf{w})) = 2\left(\frac{s_{d-1}}{3s_d}\pi^2\|\mathbf{w}\|^{-3}(1+O(\|\mathbf{w}\|^{-2}))\right)^d \quad (64)$$

when $\|\mathbf{w}\| \to \infty$. This completes the proof of Lemma 1.

a) Asymptotics for the ball $\mathcal{B}_d$.: Here, we complete the proof of the asymptotics for the ball. We study the case where feature $\mathbf{x}_t$ is uniformly distributed inside the unit ball $\mathcal{B}_d$ of dimension d. In this case the vector $\mathbf{x}$ such that $\langle \mathbf{ux}\rangle = \cos(\theta)$ satisfies the decomposition $\mathbf{x} = \cos(\theta)\mathbf{u} + \sin(\theta)\mathbf{b}$ where $\mathbf{b}$ is uniformly distributed inside the unit ball of dimension $d-1$ orthogonal to $\mathbf{u}$. Thus

$$\lambda(\mathbf{w}) = \frac{1}{v_d}\int_0^\pi \cos(\theta)^2\sin(\theta)^d v_d f(\cos(\theta)\|\mathbf{w}\|)d\theta \quad (65)$$

where v_d is the volume of the unit ball in dimension d (in fact $v_d = s_d/d$). Therefore,

$$\begin{aligned}\mu(\mathbf{w}) &= \frac{1}{v_d}\int_0^\pi \sin(\theta)^d f(\cos(\theta)\|\mathbf{w}\|)d\theta\int_{\|\mathbf{b}\|=1}\langle \mathbf{vb}\rangle^2 d\mathbf{b}. &(66)\\ &= \frac{1}{v_d}\int_0^\pi \sin(\theta)^d f(\cos(\theta)\|\mathbf{w}\|)d\theta\int_0^1 s_{d-1}\frac{r^2}{d-1}r^{d-2}dr &(67)\\ &= \frac{v_{d-1}}{v_d}\int_0^\pi \frac{\sin(\theta)^d}{d+1}f(\cos(\theta)\|\mathbf{w}\|)d\theta. &(68)\end{aligned}$$

Using $\sqrt{\det(\bar{\mathbf{B}}(\mathbf{w}))} = \sqrt{\lambda(\mathbf{w})(\mu(\mathbf{w}))^{d-1}}$, all computations done with an extra factor $\left(\frac{d}{d-1}\right)^{d/2}\left(\frac{d-1}{d+1}\right)^{\frac{d-1}{2}}$, we find at the end

$$\int \sqrt{\det(\mathbf{B}(\mathbf{w}))}d\mathbf{w} \sim (\pi/8)^{d/4}e^{-1/8}(d/4)^{-d/2} \tag{69}$$

which establishes (28).

We provide here more details of the error term as expressed in (38).

Theorem 4 (Error of (38)): The error term of the Shtarkov sum (36) is

$$O\left(\frac{d^{3/2}}{\sqrt{T\lambda(\mathbf{w}^*)^3}}\right)$$

where $\lambda(\mathbf{w}^*)$ is the is the main eigenvalue of $\bar{\mathbf{B}}(\mathbf{w}^*)$ at $\mathbf{w}^*$.

Proof: The integral (37) is asymptotically approximated by the the multidimensional Laplace method that leads to the error term estimation. We use the following change of variable $\mathbf{x} = \sqrt{\nabla^2 L_T(\mathbf{w}^*)}\mathbf{w}$

$$\int_{\Im(\mathbf{w})=-\mathbf{w}^*} \exp\left(L_T(\mathbf{w}) - \langle \mathbf{w}, \mathbf{G}_T(\mathbf{w}^*)\rangle\right) d\mathbf{w} = \frac{\exp(L_T(\mathbf{w}^*) - \langle \mathbf{w}^*, \mathbf{G}_T(\mathbf{w}^*)\rangle)}{(2\pi)^d\sqrt{det(\nabla^2 L_T(\mathbf{w}^*))}}$$
$$\times \int_{\mathbf{R}^d} \exp\left(-\frac{1}{2}\|\mathbf{x}\|^2 + O(L_T^{(3)}(\mathbf{w}^*)\|(\sqrt{\nabla^2 L_T(\mathbf{w}^*)})^{-1}\mathbf{x}\|^3)\right)$$

where $L_T^{(3)}(\mathbf{w}^*)$ is an estimate of the norm the third derivative applied to $L_T(\mathbf{w}^*)$, and is of order $O(T)$. Using the fact that

$$\|(\sqrt{\nabla^2 L_T(\mathbf{w}^*)})^{-1}\mathbf{x}\| \leq \frac{\|\mathbf{x}\|}{\sqrt{T\lambda(\mathbf{w}^*)}}$$

where $\lambda(\mathbf{w}^*)$ is the main eigenvalue of $\nabla^2 L_T(\mathbf{w}^*)$, we find

$$\int_{\Im(\mathbf{w})=-\mathbf{w}^*} \exp\left(L_T(\mathbf{w}) - \langle \mathbf{w}, \mathbf{G}_T(\mathbf{w}^*)\rangle\right) d\mathbf{w} = \frac{\exp(L_T(\mathbf{w}^*) - \langle \mathbf{w}^*, \mathbf{G}_T(\mathbf{w}^*)\rangle)}{(2\pi)^d\sqrt{\det(\nabla^2 L_T(\mathbf{w}^*))}}$$
$$\times \int_{\mathbf{R}^d} \exp\left(-\frac{1}{2}\ |\mathbf{x}\|^2\right)\left(1 + O(\frac{\|\mathbf{x}\|^3}{\sqrt{T\lambda(\mathbf{w}^*)^3}})\right).$$

But we know that for $a > 0$

$$\int_{R^d} \|x\|^3 \exp(-a\|x\|^2) = 1/a^{(d+3)/2}\pi^{d/2}\frac{\Gamma(d/2+3/2)}{\Gamma(d/2)}, \tag{70}$$

thus we conclude that

$$\int_{\mathbf{R}^d} \exp\left(-\frac{1}{2}\|\mathbf{x}\|^2\right) O(\frac{\|\mathbf{x}\|^3}{\sqrt{T}})d\mathbf{x} = O\left(\frac{\Gamma(d/2+3/2)}{\Gamma(d/2)\sqrt{T}}\right). \tag{71}$$

To complete, we observe that $\frac{\Gamma(d/2+3/2)}{\Gamma(d/2)} \sim (d/2)^{3/2}$ when $d \to \infty$. ■

We now write

$$L_T(\mathbf{W}) = \sum_t \log(1 + \sum_{k=1}^{m-1} e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_k\rangle}.$$

Since $\nabla\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_k\rangle = \mathbf{x}_t \otimes \mathbf{e}_k^\tau$, we find that $G_T(\mathbf{W}) = \nabla_{\mathbf{W}} L_T(\mathbf{W})$ has the following expression which is a $d(m-1)$ matrix:

$$\sum_t \frac{1}{1 + \sum_k e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_k\rangle}} \sum_{\ell=1}^{m-1} e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_\ell\rangle}\mathbf{x}_t \otimes \mathbf{e}_\ell^\tau = \mathbf{x}_t \otimes \mathbf{p}^\tau. \tag{72}$$

The value $\mathbf{W}^*$ that maximizes $P(\mathbf{W}, y^T)$ satisfies $\mathbf{G}_T(\mathbf{W}^*) = \mathbf{A}$ where

$$\mathbf{A} = \sum_{y_t > 0} \mathbf{x}_t \otimes \mathbf{e}_{y_t}^\tau. \tag{73}$$

Notice that $\mathbf{A}$ is now a matrix of dimension $d \times (m-1)$. We let $\mathcal{A}_T$ be the set of attainable values of $\mathbf{A}$ and we define the measure ρ_T as in the case of $m = 2$. This naturally leads to the following expression

$$r_T^*(\mathbf{x}^T) = \frac{d(m-1)}{2}\log\frac{T}{2\pi} + \log\left(\int_{\mathbf{R}^{d(m-1)}} \sqrt{\det(\frac{1}{T}\nabla^2 L(\mathbf{W}))}d\mathbf{W}\right) + O((md)^{3/2}/\sqrt{T}). \tag{74}$$

Now it remains to find the expression for $\nabla^2 L_T(\mathbf{W}) = \nabla G_T(\mathbf{W})$. We have

$$\begin{aligned}
\nabla G_T(\mathbf{W}) &= \sum_{t=1}^{T} \frac{1}{1+\sum_k e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_k\rangle}} \sum_{\ell=1}^{m-1} \nabla e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_\ell\rangle} \otimes \mathbf{x}_t \otimes \mathbf{e}_\ell^\tau \\
&\quad - \frac{1}{(1+\sum_k e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_k\rangle})^2} \left(\sum_{\ell=1}^{m-1} e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_\ell\rangle} \mathbf{x}_t \otimes \mathbf{e}_\ell^\tau \right) \otimes \left(\sum_{\ell=1}^{m-1} e^{\langle \mathbf{x}_t, \mathbf{W}\mathbf{e}_\ell\rangle} \mathbf{x}_t \otimes \mathbf{e}_\ell^\tau \right) \\
&= \mathbf{x}_t \left(\otimes \sum_k p_k(\mathbf{x}_t^\tau \mathbf{W}) \mathbf{e}_k \otimes \mathbf{e}_k \right) \otimes \mathbf{x}_t - \mathbf{x}_t \otimes \mathbf{p}(\mathbf{x}_t^T \mathbf{W}) \otimes \mathbf{p}(\mathbf{x}_t^T \mathbf{W}) \otimes \mathbf{x}_t \\
&= \mathbf{x}_t \otimes \left[\mathrm{Diag}(\mathbf{p}(\mathbf{x}_t^\tau \mathbf{W}) - \mathbf{p}(\mathbf{x}_t^T \mathbf{W}) \otimes \mathbf{p}(\mathbf{x}_t^T \mathbf{W}) \right] \otimes \mathbf{x}_t,
\end{aligned}$$

and this completes the proof.

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