ONLINE POSITRON EMISSION TOMOGRAPHY BY ONLINE PORTFOLIO SELECTION

Yen-Huan Li

Department of Computer Science and Information Engineering
Department of Mathematics
National Taiwan University

ABSTRACT

The number of measurement outcomes in positron emission tomography (PET) is typically large, rendering signal reconstruction computationally expensive. We propose an online algorithm to address this computational issue. The per-iteration computational complexity of the proposed algorithm is independent of the number of measurement outcomes and linear in the signal dimension. The algorithm has a rigorous $O(1/\sqrt{k})$ convergence rate guarantee, where k denotes the iteration counter. Numerical experiments on synthetic data-sets show that the algorithm can be significantly faster than expectation maximization and stochastic primal-dual hybrid gradient method. The proposed algorithm is based on an equivalent stochastic optimization formulation, the Soft-Bayes algorithm for online portfolio selection, and standard online-to-batch conversion.

Index Terms— Positron emission tomography, stochastic optimization, online portfolio selection, Soft-Bayes, online-to-batch conversion.

1. INTRODUCTION

Positron emission tomography (PET) is a classical task in medical imaging and plays an important role in cancer diagnoses and treatments. In its mathematical model, the measurement outcomes (numbers of detected particles) are independent Poisson random variables whose expectations depend on the unknown signal. The standard approach is then to reconstruct the signal by maximum-likelihood estimation. The negative log-likelihood function is convex, so maximum-likelihood estimation amounts to solving a convex optimization problem.

To solve the optimization problem is computationally challenging. As observed by [1], the number of measurement outcomes is typically very large in PET. Therefore, computing the full gradient—the sum of the gradients of individual log-likelihood functions—can take a lot of time. This fact renders standard convex optimization algorithms, such as gradient descent and Newton's method, slow in practice.

The issue discussed is not specific to PET, but common in modern machine learning applications. In deep learning, for example, the issue is addressed by stochastic gradient descent (SGD). SGD is an *online* algorithm that takes one or a few, instead of all, data points in an iteration, thereby circumventing full gradient computations. If the objective function satisfies standard regularity conditions, then the convergence speed of SGD is proved to be comparable to that of gradient descent in expectation.

Can we directly apply SGD to PET? To answer the question, we need to check if the log-likelihood function satisfies the regularity conditions. Existing regularity conditions require the k-th order derivative of the objective function to be bounded, for some positive integer k (see, e.g., [2]). It was proved in [3, 4] that, unfortunately, the regularity conditions do not hold in PET. The log-likelihood function involves a logarithmic loss, so its derivatives of all orders are not bounded.

Online portfolio selection is a classic problem in the field of online learning [5]. Its mathematical formulation asks one to minimize a sum of logarithmic losses by an online algorithm, similar to the online PET problem we would like to solve. There have been several attempts to address the lack-of-regularity issue in online portfolio selection; see [6] for an up-to-date list of relevant literature. However, the log-likelihood function of PET is not exactly a sum of logarithmic losses, so existing online portfolio selection algorithms are not directly applicable for our purpose.

In this paper, we show how to adapt any online portfolio selection algorithm to get an online PET algorithm. Then, we propose an explicit online PET algorithm, based on an online portfolio selection algorithm called Soft-Bayes [7]. The proposed algorithm achieves the following.

- The per-iteration computational complexity is linear in the parameter dimension and independent of the number of measurement outcomes.
- The expected numerical error provably vanishes at an $O(1/\sqrt{k})$ rate for an equivalent optimization reformulation of PET, where k denotes the iteration counter.

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Numerical results show that, on synthetic data, the proposed algorithm outperforms expectation maximization and the stochastic primal-dual hybrid gradient method.

We will focus on theoretically guaranteed online algorithms for PET in this paper. Therefore, for example, we will ignore ordered-subset expectation maximization [8] and recent deep learning-based approaches. We will also ignore the ordered-subset mirror descent algorithm [9]; in general, the log-likelihood function is not Lipschitz, so its convergence guarantee does not apply.

2. RELATED WORK

The standard approach to PET is expectation maximization. Interestingly, its convergence proof is based on Csiszár's alternating minimization framework [10, 11, 12], instead of convex analysis; the reason is perhaps the lack-of-regularity issue we have discussed in Section 1.

It is until very recently that convex optimization algorithms theoretically guaranteed for PET were developed. SCOPT, the Frank-Wolfe method, and Bregman proximal gradient method were proved to converge for PET in [13], [14], and [3], respectively. Unfortunately, they are very slow empirically, as shown in [15] for an optimization problem similar to PET. The relative SGD method proposed in [16] also converges for PET, but it involves unspecified parameters that have to be fine-tuned in practice. The stochastic primal-dual hybrid gradient (PDHG, aka Chambolle-Pock) method was developed in [17] for PET. The stochastic PDHG method is online; however, its convergence guarantee is in terms of the primal-dual gap, difficult to interpret, and its empirical speed is slow, as will be shown in Section 6.

To the best of our knowledge, the state-of-the-art algorithm for online portfolio selection is ADA-BARRONS proposed very recently [6]; it converges fast in terms of the number of iterations, but its per-iteration computational complexity does not scale well with the signal dimension, which is usually high in PET. Therefore, we consider Soft-Bayes [7], another recently proposed online portfolio selection algorithm, in this paper. Soft-Bayes converges slower than ADA-BARRONS in terms of the number of iterations but has much lower per-iteration computational complexity. Empirically, indeed, we found the performance of Soft-Bayes comparable to those of other existing algorithms on real and synthetic stock data.

3. EQUIVALENT FORMULATION OF PET

Denote by $\mathbb{R}_+$ the set of non-negative real numbers. Let $x^\natural \in \mathbb{R}_+^d$ be the unknown signal. The measurement outcomes in PET are statistically independent Poisson random variables $y_1, \dots, y_n$, such that

$$\mathsf{E}\, y_i = \langle a_i, x^\natural \rangle, \quad \forall 1 \leq i \leq n,$$

where $a_1, \dots, a_n \in \mathbb{R}_+^d$ are determined by the measurement setup. It is easily checked that the maximum-likelihood estimator of $x^\natural$ is given by

$$\hat{x} \in \operatorname*{arg\,min}_{x \in \mathbb{R}_+^d} \sum_{i=1}^n \left(\langle a_i, x \rangle - y_i \log \langle a_i, x \rangle \right).$$

As the inner product $\langle a_i, x \rangle$ can be arbitrarily close to zero, the derivatives of all orders of the term $-y_i \log \langle a_i, x \rangle$ can be arbitrarily large. Hence, the log-likelihood function violates the regularity conditions.

For any vector v, denote by $v^{(j)}$ its j-th element. By the optimality condition, Ben-Tal et al. showed the maximum-likelihood estimator can be equivalently formulated as [9]

$$\hat{z} \in \operatorname*{arg\,min}_{z \in \Delta} \frac{1}{Y} \sum_{i=1}^n \left(-y_i \log \langle b_i, z \rangle \right), \quad \hat{x}^{(j)} = \frac{Y z_j}{\sum_{i=1}^n a_i^{(j)}}, \tag{1}$$

where Δ denotes the probability simplex in $\mathbb{R}^d$, Y denotes the sum of y_i, and b_i are given by

$$b_i^{(j)} := \frac{Y a_i^{(j)}}{\sum_{i=1}^n a_i^{(j)}}. \tag{2}$$

We have deliberately introduced a scaling factor $(1/Y)$; the reason will become obvious soon.

Let I be a random variable satisfying

$$\mathsf{P}\left(I = i \right) = \frac{y_i}{Y}, \quad \forall 1 \leq i \leq n. \tag{3}$$

Then, we can write $\hat{z}$ equivalently as

$$\hat{z} \in \operatorname*{arg\,min}_{z \in \Delta} \mathsf{E}_I \left[-\log \langle b_I, z \rangle \right].$$

This reformulation of the maximum-likelihood estimator motivates us to consider online portfolio selection algorithms.

4. ONLINE PORTFOLIO SELECTION AND ONLINE-TO-BATCH CONVERSION

Online portfolio selection is a sequential game between INVESTOR and MARKET [5]. The game consists of T rounds. In the t-th round, INVESTOR announces a probability vector $w_t \in \mathbb{R}^d$, following which INVESTOR distributes the current wealth to d stocks; then, MARKET announces a vector $r_t \in \mathbb{R}^d$, which lists the price relatives of the d stocks in the t-th round. Regarding the Kelly criterion [18], the loss encountered by INVESTOR in the t-th round is defined as $-\log \langle r_t, w_t \rangle$. Both players can be strategic and make decisions based on history, i.e., those r_t and w_t that have been announced. The goal of INVESTOR is to achieve a small *regret*, given by

$$R_T := \sum_{t=1}^T \left(-\log \langle r_t, w_t \rangle \right) - \min_{w \in \Delta} \sum_{t=1}^T \left(-\log \langle r_t, w \rangle \right),$$

for any sequence of the price relatives that may adapt to the history. We say an online portfolio selection algorithm is satisfactory if it achieves $R_T = o(T)$, called a sub-linear regret in literature.

Suppose $r_1, \dots, r_T$ are statistically independent random variables. Define $G(w) \coloneqq \mathsf{E}\,[-\log \langle r_1, w \rangle]$. Given an online portfolio selection algorithm, we can transform it into an online algorithm minimizing G on the probability simplex by the following theorem.

Theorem 1 (Online-to-batch conversion [19, 20]) *Fix an online portfolio selection algorithm. Suppose the algorithm achieves $R_T \leq \gamma_T$ for some real number γ_T. Let $w_1, \dots, w_T$ be the algorithm's outputs, and $\bar{w}_T$ be the time average of $w_1, \dots, w_T$. Then, it holds that*

$$\mathsf{E}\, G(\bar{w}_T) - \min_{w \in \Delta} G(w) \leq \frac{\gamma_T}{T},$$

where the expectation is with respect to the random variables $r_1, \dots, r_T$. □

If the algorithm achieves a sub-linear regret, then any numerical error requirement can be achieved with a sufficiently large T. Suppose the online algorithm is *anytime*; that is, the algorithm does not have any parameter dependent on T. Then, one gets

$$\mathsf{E}\, G(\bar{w}_t) - \min_{w \in \Delta} G(w) \leq \frac{\gamma_t}{t}, \quad \forall t \in \mathbb{N},$$

where $\bar{w}_t$ denotes the time average of $w_1, \dots, w_t$, and γ_t is a regret bound for the first t rounds.

5. PET BY STOCHASTIC SOFT-BAYES

By the results in the preceding two sections, any online portfolio algorithm can be transformed for online PET as the following. Suppose the algorithm is anytime for convenience, which is indeed the case for Soft-Bayes. Let $z_1 = (1/d, \dots, 1/d) \in \Delta$ and

$$x_1^{(j)} = \frac{Y}{d \sum_{i=1}^n a_i^{(j)}}. \tag{4}$$

Recall that Y was defined in Section 3. In the t-th iteration, we sample a random index i_t following (3) independent of the past; then, we call the online portfolio selection algorithm with b_{i_t} and set z_{t+1} as the output; finally, we set the $(t+1)$-th iterate x_{t+1} as

$$x_{t+1}^{(j)} = \frac{Y \bar{z}_{t+1}^{(j)}}{\sum_{i=1}^n a_i^{(j)}}, \tag{5}$$

where $\bar{z}_{t+1}$ denotes the time average of $z_1, \dots, z_{t+1}$. We emphasize that the procedure above is valid for any online portfolio selection algorithm that is anytime and achieves a sub-linear regret.

Algorithm 1 Stochastic Soft-Bayes

Set $z_1 = \bar{z}_1 = (1/d, \dots, 1/d)$.
Compute x_1 as in (4).
for $t \in \mathbb{N}$ **do**
  Sample i_t following (3), independent of the past.
  Set $\eta_t = \sqrt{(\log d)/(2dt)}$.
  Compute $z_{t+1} = (1 - \eta_t) z_t + \eta_t \frac{b_{i_t} \cdot z_t}{\langle b_{i_t}, z_t \rangle}$.
  Compute $\bar{z}_{t+1} = (t \bar{z}_t + z_{t+1}) / (t+1)$.
  Compute x_{t+1} as in (5).
end for

As discussed in Section 2, we choose Soft-Bayes as the online portfolio selection algorithm to balance between regret and computational complexity. We call the resulting algorithm Stochastic Soft-Bayes in the rest of the paper, for convenience of presentation. We summarize the algorithm in Algorithm 1, where the notation $\cdot$ denotes element-wise multiplication.

Obviously, the per-iteration computational complexity of Stochastic Soft-Bayes is $O(d)$, independent of the number of measurement outcomes n. This is arguably the lowest per-iteration computational complexity one can expect, as d is the signal dimension. Soft-Bayes achieves $R_t = O(\sqrt{T d \log d})$ for any $t \in \mathbb{N}$. By Theorem 1, the regret bound translates into the following convergence guarantee for PET.

Proposition 1 *The sequence $(x_t)_{t \in \mathbb{N}}$ converges to a maximum-likelihood estimate. Moreover, for the equivalent formulation* (1) *of PET, it holds that*

$$\mathsf{E}\, f(\bar{z}_t) - \min_{z \in \Delta} f(\bar{z}_t) = O\left(\sqrt{\frac{d \log d}{T}} \right),$$

where f denotes the objective function in (1)*, i.e.,*

$$f(z) \coloneqq \frac{1}{Y} \sum_{i=1}^n \left(-y_i \log \langle b_i, z \rangle \right).$$

□

6. NUMERICAL EXPERIMENTS

In this section, we compare the performance of the proposed algorithm, Stochastic Soft-Bayes, with those of expectation maximization and the stochastic PDHG method. As discussed in Section 2, there are other algorithms that provably converges for PET. However, they are too slow in practice or involve unspecified parameters, so we exclude them.

The numerical experiments were done using the Julia language, on a MacBook Pro with 2.5GHz Intel Core i7 Processor and 16GB DDR3 memory. We use a synthetic data-set generated by the Poisson noise model in Section 3. The true signal to be reconstructed consists of three rectangular functions of different widths, as a toy one-dimensional analogue

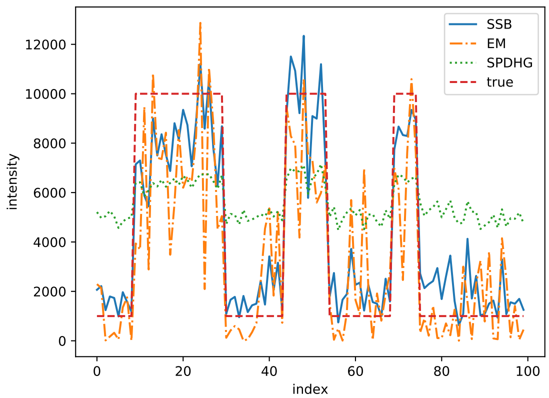

Fig. 1. Reconstructed and true signals.

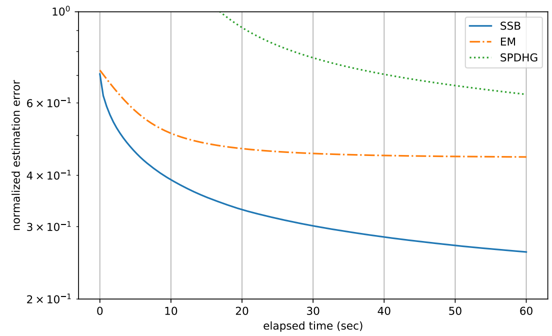

Fig. 2. Normalized estimation errors with respect to the elapsed time in seconds.

of typical test images in PET. The signal dimension d equals 100, and the number of measurement outcomes n is set to 100000. The widths of the three rectangular functions are 5, 10, and 20, respectively. The vectors a_i are generated following the scheme in [21]. Expectation maximization and Stochastic Soft-Bayes are parameter-free; for the stochastic PDHG method, we set the parameters as in [17], except that we take only one data point in every iteration.

We report the results after running each of the three algorithms for one minute in Figure 1–3. In the figures, SSB denotes Stochastic Soft-Bayes, EM denotes expectation maximization, and SPDHG denotes the stochastic PDHG method. Figure 1 shows the reconstructed and true signals. We can observe that SSB achieves a better contrast than the other two methods. Figure 2 shows the normalized estimation errors in terms of the elapsed time on the MacBook Pro in seconds. The normalized estimation error is defined as the estimation error in the ℓ_2-norm divided by the ℓ_2-norm of the true signal. Figure 3 shows the normalized estimation errors in terms of the number of epochs. An epoch is defined as one pass of the whole data-set; therefore, one epoch corresponds to one iteration for EM, and n iterations for SSB and SPDHG (though n iterations do not necessarily imply one pass of the data-set, as the data points are randomly chosen). We can observe that SSB achieves the best performances in the three figures.

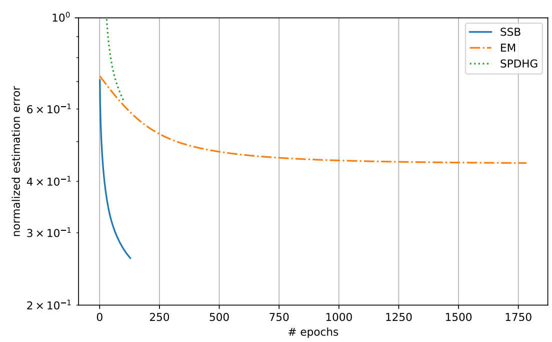

Fig. 3. Normalized estimation errors with respect to the number of epochs.

7. CONCLUDING REMARKS

In this paper, we have shown how to design an online PET algorithm given an online portfolio selection algorithm. We have proved a non-asymptotic convergence guarantee for the resulting online PET algorithm. We have used Soft-Bayes to construct an explicit instance, which achieves the best performances in our numerical experiments.

We notice the statistical model of PET also appears in a variety of applications [22, 23], to which our framework directly applies. In applications where the parameter dimension is moderate, one may want to adopt ADA-BARRONS, instead of Soft-Bayes, to achieve a faster convergence rate whenever the per-iteration computational complexity is still acceptable.

Two research problems immediately follow. First, the non-asymptotic convergence guarantee in Proposition 1 is for the numerical error in the equivalent optimization formulation (1). Is it possible to translate the guarantee or derive another guarantee for the error in the original negative log-likelihood function? Second, what we have developed is an online algorithm for maximum-likelihood estimation. Is it possible to develop an online algorithm that directly minimizes the expected negative log-likelihood function? Such an algorithm is desirable, as its numerical error corresponds exactly to the statistical error.

The setup in our numerical experiments is far from realistic. We are working on testing the proposed algorithm on real data-sets.

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