HOW TO SAMPLE IF YOU MUST: ON OPTIMAL FUNCTIONAL SAMPLING

Assaf Hallak
Shie Mannor

Abstract. We examine a fundamental problem that models various active sampling setups, such as network tomography. We analyze sampling of a multivariate normal distribution with an unknown expectation that needs to be estimated: in our setup it is possible to sample the distribution from a given set of linear functionals, and the difficulty addressed is how to optimally select the combinations to achieve low estimation error. Although this problem is in the heart of the field of optimal design, no efficient solutions for the case with many functionals exist. We present some bounds and an efficient sub-optimal solution for this problem for more structured sets such as binary functionals that are induced by graph walks.

Keywords: Learning Theory, Other Applications.

1. Introduction

Consider a network in which each link has a delay characterized with some parametric distribution. The network can be probed in order to find an estimator for these parameters, yet the only measurement obtained for each probe is the sum of delays along the path. As each probe costs time, efficiently sampling the network is crucial for estimating the delays accurately. This example is one of many that can be modeled by the generative model studied in this paper:

Problem 1. Define the following system: N is the number of variables, $x_t \in \mathbb{R}^N$ is the sample at stage t, y_t is the measurement produced in the following manner:

$$y_t = w_t^\top x_t, \quad w_t \sim N\left(\mu, diag\left\{\sigma_i^2\right\}_{i=1}^N\right),$$

where σ_i^2 are known. At each stage one may choose x_t from a certain subset $X \subseteq \mathbb{R}^N$, observe y_t and then find an estimator $\hat{\mu}$ using the history of the samples. The problem is how to choose x_t such that the estimator will have as low error as possible.

To better understand the problem, we revisit the network tomography problem ([**?**, **?**]):

Example 2. Observe the following network:

Assume that moving through each link in the network results in a random delay $w(e_i) \sim N(\mu_i, 1)$. The possible traces one can probe must start and end in a computer, so only the traces $C_1 \to H \to C_2$,$C_1 \to H \to C_3$, $C_2 \to H \to C_3$ and the reverse traces are available. These can yield the following samples $w(e_1) + w(e_2), w(e_1) + w(e_3), w(e_2) + w(e_3)$. After sampling once from each trace, it is possible to estimate μ_1, μ_2 and μ_3 with finite expected error. Drawing more samples will yield an estimator with lower error, but how should one draw them? Assume

for instance $C_1 \to H \to C_2$ is sampled more frequently than the other traces. This may result in a lousy estimator for μ_3 since this probe does not include e_3. If the error in each estimator is equivalently important to us, the optimal policy in this case is not surprisingly probing the network uniformly over the available traces. However, generally uniform sampling can generate terrible results.

The paper consists of the following parts: in the next section we survey previous related works in several fields such as experiment design, learning theory and network tomography. In Section 3 we formulate the problem and discuss its known solution and mathematical properties. In the succeeding sections, special structured functionals sets will be considered: initially the general binary case, and afterward sets generated by graph walks. In graph walks we discuss two setups: in the first, the random variables are associated with the nodes, and in the second setup, they are associated with the edges in the graph (like in Example 2). In Section 7 we point out the relation to recent works on a specific bandit setup. The final chapter will present conclusions, as well as suggestions, for the ongoing research.

2. Previous work

Similar generative models as posed in Problem 1 have been widely studied in the field of optimal design (see Pukelsheim [**?**] for an overview of the field). However, as the size of the finite set X grows, common solutions such as SDP solvers and gradient techniques are insufficient as their complexity depends on the set size. This difficulty is recognized in network tomography where each functional is identified with a trajectory on the graph so that the size of X can be exponential in the number of variables. Our work suggests an efficient solution for this particular case.

In machine learning the field of active learning is concerned with similar problems (for a survey see [**?**]). Problem 1 highly resembles the multiple linear regression model [**?**], however unlike regression our work is not focused on estimating the parameters but rather on choosing samples that will result in a better estimator. For example, Cohn et al. [**?**] have studied optimal active learning in various models, including the kernelized weighted least squares setup. Despite the similarities between the problems, several key differences in the setup had led to entirely different mathematical formulations. Our focus is on using the structure of the set X for obtaining an efficient sampling strategy that minimizes the estimation error.

We observe an interesting connection to exploration in bandit problems through the work of Dani et al. [**?**] and its follow-up by Cesa-Bianchi and Lugosi [**?**]. They have come across a key problem similar to ours while proving bounds on the exploration component of the adversarial online bandit problem with a restricted linear sampling set. Although these works took great interest in assessing a similar value function to the one we later present, their work did not address the optimal sampling issue addressed by us, nor the computational effort in finding it. As an application of our work, we solve a specific example mentioned in [**?**].

The main application presented here concerns "Network Tomography" (coined by Vardi [**?**]), which deals with inference on the parameters or topology of a network through probing (for an overview see Coates et al. [**?**]). In this field there are many interesting setups, for example finding a network's structure or some of its unique properties [**?**, **?**, **?**]. For instance, in a recent work, Thouin et al. suggested using active learning in order to infer the bandwidth of a network ([**?**]). Another

related work on parameter estimation was done by Tsang [?] who addressed the same problem with different parameters and stresses. However, most of the works in the field have dealt with more complicated distributions in different schemes and most of the efforts were put into finding efficient computation of fine estimators [?, ?, ?] rather than on how to best probe the network.

3. The unconstrained problem

In the introduction we presented Problem 1: how to choose x_t in order to minimize the error of the estimators. After observing another example we shall examine the model more closely:

Example 3. Define the following problem:

$$X = \{(1,1,3),(1,1,0),(-2,-2,5)\},\ w \sim N\left((\mu_1,\mu_2,\mu_3), diag\,(1,1,2)\right)$$

In this example, it is possible to sample at each time step one of the following linear combinations: $w(1)+w(2)+3w(3)$, $w(1)+w(2)$, $-2w(2)-2w(2)+5w(3)$.

Apparently, not all entries of μ can always be estimated with a finite error: since all possible linear combinations include some multiplication of the expression $w(1)+w(2)$, adding a constant to μ_1 and subtracting it from μ_2 will not change the probability of the measurements and therefore is undetectable, which implies a possibly infinite estimation error for each. While the most logical way of handling this situation here might be defining a new variable $\tilde{w}_{1,2} = w(1)+w(2)$, in more complex cases it is not entirely clear how new variables should be defined. Therefore, throughout the rest of the paper, unless specified otherwise, we shall assume this situation does not occur, however it still must be taken into account.

Since all the variables in this model form a normal multivariate vector, finding the MVUE (Minimum Variance Unbiased Estimator) which is also the MLE (Maximum Likelihood Estimator) [?] $\hat{\mu}$ is straightforward. Let Γ be the $T \times N$ matrix whose t^{th} row is x_t, $\sigma_{F,t}^2 = x_t^\top diag\left(\sigma_i^2\right)_{i=1}^N x_t$ is the variance of the t^{th} functional and Σ_Γ is the diagonal matrix $\Sigma_\Gamma = diag\left(\sigma_{F,t}^2\right)_{t=1}^T$. The following proposition is taken from Pukelsheim [?]:

Proposition 4. *The inverse Fisher information matrix which is also the MSE matrix for the MVUE estimator is given by:*

$$MSE(\mu) \triangleq E(\mu-\hat{\mu})(\mu-\hat{\mu})^\top = M^{-1} \triangleq \left(\sum_{t=1}^T \frac{1}{\sigma_{F,t}^2} x_t x_t^\top\right)^{-1} = \left(\Gamma^\top \Sigma_\Gamma^{-1} \Gamma\right)^{-1}.$$

As the MSE is a matrix, we would like to choose some scalar scoring function to minimize. There are several suitable options (see Pukelsheim [?]), but we believe the simplest analytically and most appropriate option is finding A-optimality, i.e. minimizing the trace of the estimator's covariance matrix M^{-1}.

Instead of solving the discrete time setup, we shall identify the optimal decision policy as some stationary distribution on X . To ease the notation we will assume from now on that the random variables have unit variance (i.e. $w_t(i) \sim N(\mu_i, 1)$). In addition, we shall restrict X to be a finite set for tractability reasons. Denote by Δ_N the simplex set in N variables, i.e. $\Delta_N = \left\{v \in \mathbb{R}_+^N | \mathbf{1}^\top v = 1\right\}$. The problem can be formulated as follows:

Problem 5. Find the optimal distribution P on linear combinations from X that achieves:

$$P = \arg\min_{P\in\Delta_N} tr\left(\left[\sum_{x\in X}\frac{p(x)}{x^\top x}xx^\top\right]^{-1}\right).$$

Remark 6. Pukelsheim [**?**] and Cesa-Bianchi and Lugosi [**?**] have formulated a different problem for which the factor $\frac{1}{x^\top x}$ does not appear in each summand. This is due to the slightly different setup: Pukelsheim had defined that samples have the same variance for each functional, while in our setup it is constant per coordinate, but functional dependent.

To simplify notation from now on, we abuse our previous notation by redefining Γ as the $|X|\times N$ matrix whose rows are the distinct $x\in X$. Moreover, we define the matrices $L = diag\left(x^\top x\right)_{x\in X}$ and $P = diag\left(p(x)\right)_{x\in X}$ so $M = \Gamma^\top L^{-1}P\Gamma$, and we want to minimize $tr\left(M^{-1}\right)$. Evidently Problem 5 can be fitted in a standard form as seen in [**?**].

Corollary 7. *$Tr\left(M^{-1}\right)$ is a convex function of $p(x)$ and Problem 5 can be solved using SDP (Semi-Definite Programming).*

Remark 8. There is a minor variation on Problem 5 that can be handled similarly: consider the same objective function, only that now each functional x is associated with a cost $c(x)$ and there is some restricted budget C. Adding the linear constraint $\sum_{x\in X} c(x)\,p(x)\le C$ to the formulation does not affect its solvability using SDP.

According to Corollary 7, solving Problem 5 can be done in polynomial time as a function of $|X|$. However, when X is very large it is unfeasible. Nevertheless, in practice large sampling spaces tend to contain some inner structure and this is our motivation. We view graph walks as structured sets for which a sub-optimal yet efficient solution is employed.

4. Binary functionals

Binary functionals, i.e., linear combinations with coefficients only in $\{0,1\}$, are an important and interesting subset of possible functionals, since they are sufficient to describe sampling in special models such as graphs. The meaning of using binary functionals is that you choose which of the N elements are part of your sample. We start with the case where a subset of size K of the variables is chosen.

4.1. K-choose-N.

The most natural set of binary functionals is the set of all functionals with exactly K ones. For example, for $K=1$ we get $X=\{e_i\}_{i=1}^N$ and for $K=N$ we get $X=\{\mathbf{1}\}$ ($\mathbf{1}$ denotes the vector of N ones). It turns out the optimal solution for these sets can be found analytically, as well as the solution for unions of K-choose-N sets for different values of K.

Definition 9. Denote the K-choose-N set B_K by $B_K \triangleq \left\{x\in\{0,1\}^N \mid x^\top\mathbf{1}=K\right\}$.

The following theorem determines the optimal solution for Problem 5 when $X = B_K$:

Theorem 10. *Let $X = B_K$. The optimal solution for Problem 5 is choosing uniformly functionals over X, and the optimal MSE is given by: $tr\left(M^{-1}\right) = \frac{N}{K} + \frac{(N-1)^2 N}{N-K}$.*

Proof. First we find the trace of the uniform decision for which $M = \frac{1}{K\binom{N}{K}} \sum_{x \in B_K} xx^\top$. By applying a counting argument we obtain $M_{i,i} = \frac{1}{N}$, $M_{i,j} = \frac{K-1}{N(N-1)}$ and $tr\left(M^{-1}\right) = \frac{N}{K} + \frac{(N-1)^2 N}{N-K}$.

Now assume M is A-optimal. Due to the symmetry of B_K for each variable, for any permutation matrix Φ we have $\Phi^T M \Phi \in conv\left(B_K\right)$. From the convexity of Problem 5 we can conclude that:

$$tr\left(\left(\frac{\sum_{\Phi \in S_N} \Phi^T M \Phi}{N!}\right)^{-1}\right) \leq \frac{\sum_{\Phi \in S_N} tr\left(\left(\Phi^T M \Phi\right)^{-1}\right)}{N!} = tr\left(M^{-1}\right).$$

Due to symmetry the matrix $M' = \frac{1}{N!} \sum_{\Phi \in S_N} \Phi^T M \Phi$ has constant diagonal entries and constant off-diagonal entries denoted c_{diag}, c_{off} respectively. Since $tr\left(M'\right) = 1$ we know that $c_{diag} = \frac{1}{N}$. As $M' \in conv\left(B_K\right)$ we have $\mathbf{1}^T M' \mathbf{1} = N c_{diag} + N\left(N-1\right) c_{off} = K$, so $c_{off} = \frac{K-1}{N(N-1)}$ and M' is the same matrix obtained by uniform choice. □

Example 11. for $K = N - 1$ we get $tr\left(M^{-1}\right) = \frac{N}{(N-1)} + \left(N-1\right)^2 N$, an N^3 asymptotic behavior.

Since the best value of K is 1, and for $K = N - 1$ we got an error that scales like N^3. We generalize this notion that smaller K yields better results:

Corollary 12. *If $K_1 < K_2$, then the optimal solution of Problem 5 for $X_1 = B_{K_1}$ is smaller and therefore better than the optimal solution of Problem 5 for $X_2 = B_{K_2}$.*

Proof. Obtained from analysing $tr\left(M^{-1}\right) = \frac{N}{K} + \frac{(N-1)^2 N}{N-K}$ as a function of K. □

So far we have shown the optimal solution for N-choose-K sets, and in Corollary 12 we also show that sets with smaller K can be used better. This result can be strengthened by the subsequent theorem that suggests that if X contains several N-choose-K subsets, only the smallest subset is used for the optimal solution. In addition, it gives rise to a general lower bound on binary functionals:

Theorem 13. *Assume $X = \bigcup_{i=K}^{N} B_i$, i.e., X is the set of all linear combinations with at least K ones. The optimal solution of Problem 5 is given by a uniform choice over the functionals in B_K.*

Proof. Like we showed in the proof of Theorem 10, there is an optimal matrix M with constant off diagonal entries and due to its unit trace and symmetry its diagonal entries are $\frac{1}{N}$. The smallest off diagonal constant yields the minimal $tr\left(M^{-1}\right)$ so choosing the smallest K is optimal. □

Conclusion: For Problem 5, if $X \subseteq \bigcup_{i=K}^{N} B_i$, meaning all functionals in X have at least K ones, then $tr\left(M^{-1}\right) \geq \frac{N}{K} + \frac{(N-1)^2 N}{N-K}$.

5. Graph paths with randomness in the nodes

Given a source-drain DAG (Directed Acyclic Graph) with N inner nodes, and assume $V = \{v_s, v_d\} \bigcup \{v_i\}_{i=1}^{N}$ where the order over the nodes is defined by a topological order. Each inner node is associated with a normally distributed random

variable $w(i) \sim N(\mu_i, 1)$, with an unknown μ_i. We would like to estimate the μ_i's with minimal MSE. This scheme can model for example networks with delays generated from the networking equipment in each node, but with constant or very low variance link delays, e.g., optical networks. Denote by x both the actual path in the graph, and the corresponding characteristic vector, i.e., $x(i) = 1$ iff $v_i \in x$.

Example 14. Consider the following source-drain DAG:

The possible paths on the graph allow us to sample the following linear combinations: $w_1+w_2+w_3, w_1+w_2, w_1+w_3, w_2, w_2+w_3$, so the corresponding Γ matrix is: $\Gamma^T = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \end{bmatrix}$.

The following example exhibits many problems in the model we must take into account:

Example 15. Consider a grid graph of the following form:

This kind of graph is a good example for what can happen when ignoring the complexity of Problem 5 and instead uniformly choosing functionals from the given set: if all paths on the grid are chosen the same number of times, then the nodes in the middle will be sampled much more often than these far on the sides, since many more paths go through them. In their paper, Cesa-Bianci and Lugosi [**?**] have also addressed this counter example to the good results of uniform distribution over the trajectories of many other graphs and models. They suggested in their paper to find a better solution using semi-definite programming which is impractical for non-trivial grids.

The number of paths in the example is large, which makes finding the solution unfeasible for many nodes. Another concern we have neglected so far that emerges in this example is its identifiability: in this grid graph, adding a constant to the mean of all nodes at a certain layer (meaning all nodes at the same distance from the source) and subtracting the same constant from the mean of all nodes at another layer will not change the distribution of the samples, so the set of possible paths is unidentifiable. Apparently this is a key problem in any layers graph, and although there are some reasonable suggestions for dealing with this issue we shall neglect it in this paper as it draws us further from the main scope.

Since the number of paths can be exponential in the number of nodes, there might be too many functionals to optimally find the MSE using SDP solvers. To cope with this setback, we offer a relaxed solution that can be computed efficiently using dynamic programming. Simulations show that our approach works quite well.

5.1. **The product distribution.** We propose a relaxed solution using dynamic programming by introducing the product problem: observe only the distribution on paths generated as the product of the leaving distribution from each node. More specifically, denote $\alpha_{i,j}$ as the probability to leave the vertex v_i using the edge $e_{i,j}$, so we get the following equations: $\sum_{j=i+1}^{N} \alpha_{i,j} + \alpha_{i,d} = 1,\ p(x) = \prod_{i,j:e_{i,j}\in x} \alpha_{i,j}$. Now we can define the relaxed problem which we later show is easier to solve:

Problem 16. Find the optimal exit distributions α that solves the following problem:

$$\begin{cases} \min_{\alpha} & tr\left(\left[\sum_{x\in X}\frac{p(x)}{x^\top x}xx^\top\right]^{-1}\right) \\ \text{subject to} & p(x)=\prod_{i,j:e_{i,j}\in x}\alpha_{i,j},\ \alpha_{i,j}\geq 0,\ \sum_{j=i+1}^{N}\alpha_{i,j}+\alpha_{i,d}=1 \end{cases}.$$

Example 17. Recall the graph from Example

The value on each edge represents the exit distribution from its source node so the distribution over paths is given by:

$$p(v_s\to v_1\to v_2\to v_d)=0.7{\cdot}0.2{\cdot}0.5=0.07,\ p(v_s\to v_2\to v_3\to v_d)=0.3{\cdot}0.5{\cdot}1=0.15,...$$

Notice that the set of product distributions is a subset of all possible distributions over the paths, so the optimal product distribution may produce a much worse MSE than the optimal unconstrained distribution. However, since for optimization on the exit distributions α we got no more than N^2 variables, if M can be expressed efficiently using α then the computation effort will be drastically reduced. In order for Problem 16 to have an efficient solution we need to be able to calculate the matrix M without directly calculating $p(x)$ for each x. In Theorem 18 we show how it can be done:

Theorem 18. *The matrix $M(\alpha)$ can be computed in polynomial time using dynamic programming.*

Proof. First we show how one can compute how many times length l paths contain each node. We calculate for each node sequentially (according to a topological sort) how many times paths of length l from the source finish in this node using the following equation: $\Phi_i(l)=\sum_{j=1}^{i-1}\alpha_{j,i}\Phi_j(l-1)+\alpha_{s,i}1\{l=1\}$. Likewise, we can calculate for each node sequentially how many length l paths started in it and finished at the drain by employing the following equation: $\Theta_i(l)=\sum_{j=i+1}^{N}\alpha_{i,j}\Theta_j(l-1)+\alpha_{i,d}1\{l=1\}$. Now the number of length l paths that passed through node i is given by: $J_{i,i}(l)=\sum_{j=1}^{l-1}\Phi_i(j)\Theta_i(l-j)$. In a similar fashion we can compute the number of length l trajectories that passed through both node i and node j: $J_{i,j}(l)$. Finally, realizing that the matrix $J(l)$ satisfies $J(l)=\sum_{x:x^T\mathbf{1}=l}p(x)xx^\top$, we can compute M as the weighted sum of the matrices $\{J(l)\}_{l=1}^{N}$: $M=\sum_{l=1}^{N}\frac{1}{l}J(l)$. □

Obviously, the matrix M linearly depends on each distinct set of leaving probabilities $\{\alpha_{i,j}\}_{j=i+1}^{d}$ or entering probabilities $\{\alpha_{i,j}\}_{i=s}^{j-1}$, while not changing the other values of α. Therefore for each such set of variables the problem of minimizing $tr\left(M^{-1}\right)$ is an SDP in that specific set of variables. However, over the entire set of variables $\{\alpha_{i,j}\}$ the function is not an SDP as it is not convex. Therefore, even if we compute for each node iteratively the optimal exit distribution assuming all the other distributions are constant, we cannot be assured the solution found is globally optimal. Algorithm 1 describes this general scheme. Notice that the objective function decreases at each iteration so convergence is guaranteed. The order in which the nodes are chosen can play a role in the convergence rate; we leave that aspect for future research. Empirically the optimal solution is unique and closely approximates the solution of Problem 5, as seen in Figure 5.2 (A).

Algorithm 1 Optimize_Products

1. Start with random exit distributions for each node $\{\alpha_{i,j}\}$.
2. Choose node v.
3. Find the optimal exit distribution $\{\alpha_{v,j}\}_{j=v+1}^{d}$ from node v to all other nodes assuming all other exit distribution $\{\alpha_{i,j}\}_{i\neq v}$ are constant.
4. Go to step 2 with a different node.

In Figure 5.2 (B) we compare our relaxed solution against the uniform distribution for the grid graph. Note that for square grids with a nodes on each side there are $\begin{pmatrix} 2a-2 \\ a-1 \end{pmatrix}$ paths in the graph, so the optimal solution is impossible to compute for large a. To deal with the identifiability problem, instead of $tr\left(M^{-1}\right)$ we used the objective function $\sum_{\lambda_i \neq 0} \frac{1}{\lambda_i}$ to minimize. The results for the product distribution are much better than these obtained by the uniform distribution.

FIGURE 5.1. The optimal product distribution for 5×5 grid. Notice the weights give higher probability to go through the corners than the uniform distribution.

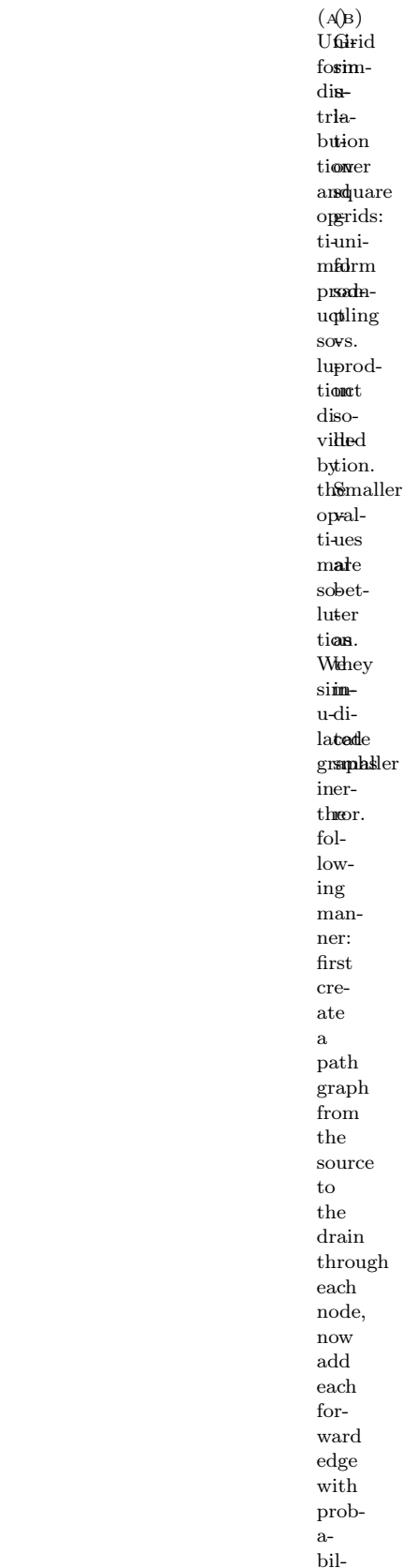
6. Graph paths with randomness on the edges

Although we initially acknowledged DAG graphs in which the randomness is associated with the vertices, it is common in application to associate them with the edges, for example as delays in a network. To fit our model to such applications we shall now assume a graph with multiple access points from which the user can probe the network to another access point. Even though such graphs will not necessarily be DAGs, we will not allow cycles as they are not usually allowed in regular networks and adversely affect the estimation since they just add more noise.

Let $G = (V, E)$ be a simple graph where each edge is associated with a normal random variable with an unknown mean and unit variance. In addition let $S \subseteq V$ be a set of access points in the graph. Each time step, it is possible to choose a path in the graph starting with one access point and ending in another. Finally, the sum of the random variables over the edges in the path is presented, from which one can estimate the expectation of the random variable associated with each edge. Although a directed graph is more appropriate to describe reality, in the next example we shall assume that the graph is undirected for simplicity, which is equivalent to the claim that the delay in each direction has the same distribution.

Example 19. Consider a star graph with v_0 as its center vertex and assume that all edges from and to the center exist. If $S = V \setminus \{v_0\}$, we get an identical case as N-choose-K, where $K = 2$. As we saw, the optimal solution here is uniform over all 2 access points. Notice that by giving uniform distribution from the center vertex to any of the edges except the one of the root access point, the optimal solution in this setting is obtained.

FIGURE 5.2. Matlab Simulations. For the implementation we used the CVX package [**?**, **?**].



In order to cope with the exponential number of paths, we can define here as well a product rule: for each node $v_i \in V$, and its set of exit edges $\{e_{i\to j}\}_{j:v_j\in \text{Neighbors}(v_i)}$ define an exit distribution $\alpha_{i\to j}$ as the probability to take the edge $e_{i\to j}$ from node v_i.

Theorem 20. *The matrix $M(\alpha)$ can be computed in polynomial time complexity using dynamic programming.*

Proof. In a similar fashion to the proof of Theorem 22 we can calculate for each access point and for each edge $e_{i\to j}$ in the graph by dynamic programming the number of k-length paths that began at that access point and ended at vertex i. Similarly we can calculate the number of k-length paths that began at vertex j and ended in that access point. Convolving the results provides us with the number of k-length paths that passed through the edge $e_{i\to j}$, and from that $M_{i\to j}$ is easily obtained. □

Theorem 20 allows us to use Algorithm 1 for efficient computation of optimal product solution for this case as well, so the product solution can be used for efficient estimation of delays in networks.

7. Online bandits

Cesa-Bianchi and Lugosi [**?**] have come across a similar problem in the adversarial online bandit problem with a restricted linear sampling set. They showed a performance bound that depends on the lowest eigenvalue of the matrix $F = \sum_{x\in X} p(x)\, xx^\top$. Maximizing the smallest eigenvalue is called in the literature E-criterion and it can be formulated in SDP form. It is easy to see that $\left(\min_{x\in X}\|x\|^2\right) M \preceq F \preceq \left(\max_{x\in X}\|x\|^2\right) M$ (using the Lowener order for symmetric matrices), and that if all vectors in X have norm b (like in the K-choose-N example or the grid) then $F = bM$. This means that there is a close connection between the two problems, especially for the binary case for which $\frac{\max_{x\in X}\|x\|^2}{\min_{x\in X}\|x\|^2} \le N$. In that case, as stated by Theorems 18 and 21, relaxed solutions can be found efficiently for Problem 5 on the graph setups by considering product distributions. For minimizing F there is a similar result as we show in the next Theorem for nodes-associated randomness (a similar result can be shown for the case of edges):

Theorem 21. *The matrix $F(\alpha)$ can be computed in polynomial time complexity using dynamic programming.*

Proof. Denote by $n(j)$ the appearance frequency of the j'th node and by $n(i,j)$ the joined appearance frequency of nodes i and j. Observe that $n(j) = \sum_{k=s}^{j-1} n(k)\,\alpha_{k,j}$, $n(i,j) = \sum_{k=i}^{j-1} n(i,k)\,\alpha_{k,j}$. So computing $F_{i,j} = n(i,j)$ is simply applying these equations in the order they are written for incrementing values of j. □

According to Theorem 21, Algorithm 1 can be used for minimizing F on all product distributions efficiently as well. Therefore we can use this algorithm to find and simulate sub-optimal exploration distribution on the sampling space in the suggested bandit setup.

8. Conclusions

In this paper we considered a fundamental problem that is common in many setups. Although a straightforward solution for the optimal sampling problem exists, it might be unfeasible to compute. Therefore, for graph paths we proposed an efficient relaxed solution that exploits the graphical structure using dynamic programming. The suggested solution was tested empirically and our simulations showed good behavior. In addition we linked a recently suggested bandit setup with the field of optimal experiments design, and employed our solution on the grid example for which uniform sampling is inadequate.

Our paper opens up some interesting research directions. Among these directions are: the case of an infinite set X, bounding the difference between the relaxed product solution and the optimal one, finding graph properties based bounds, and analyzing the behavior of random graphs or sets in this context.