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Efficient estimation of the cardinality of large data sets

Philippe Chassaing and Lucas Gerin

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Abstract

F.Giroire has recently proposed an algorithm which returns the *approximate* number of distinct elements in a large sequence of words, under strong constraints coming from the analysis of large data bases. His estimation is based on statistical properties of uniform random variables in $[0, 1]$. Here we propose an optimal estimation, using information and estimation theory¹.

1 Introduction

The aim of this note is to improve a solution proposed by Giroire [Gir05] to the following problem: consider a sequence $Y = (Y_1, \dots, Y_N)$ of words (one may think to a sequence of file on a disk, a list of requests, a novel from Shakespeare, *etc...*); we don't make any assumption on the structure of Y , and we want to know the number (usually denoted F_0 in the data base community) of *distinct* elements of this sequence. The motivation comes from analysis of large data sets, and especially analysis of internet traffic: certain attacks may be detected at router level, because they generate an unusual number of distinct connections (see [Fla04]). Most of algorithms use a dictionary to store every word, so that the memory needed is linear in F_0 . Here the size of data sets is huge, making it impossible to store every word, so that the algorithm should satisfy the two following constraints: it should use constant memory and do only one pass over the data. These constraints are very strong, but on the other hand we allow the algorithm to give only an *estimation* of F_0 .

The main idea used in [Gir05], introduced by Flajolet and Martin [FM85], is to transform this problem in a probabilistic one, using hash functions.

A *hash function* is a function $h : \mathcal{C} \rightarrow [0, 1]$, where \mathcal{C} is a finite set of words (say english language, $\{0, 1\}^8$, *etc...*) such that *the image of a typical sequence of words behaves as a sequence of i.i.d random variables, uniform in $[0, 1]$.*

This definition is of course somewhat informal, but we will assume, from now on, that, noting $X_i = h(Y_i)$, then $\mathbf{X} = \{X_1, \dots, X_N\}$ is the realization of F_0 i.i.d. r.v., uniform on $[0, 1]$. Existence and construction of *good* hash functions is discussed in [Knu73].

Set $\theta = F_0$ and denote as usually $X_{(1)}$ the smallest X_i , $X_{(2)}$ the second smallest, and so on. The key point is that the information on θ contained in $\{Y_1, \dots, Y_N\}$ is equivalent to that contained in $(X_{(1)}, \dots, X_{(\theta)})$.

As a consequence, we are now dealing with a classical statistical problem: given a (small) sample of (X_1, \dots, X_θ) , i.i.d. r.v., uniform on $[0, 1]$, we want to estimate the (large) parameter θ . Denote by M the memory available (how many real numbers that can be stored). One should determine:

1. A way of extracting a M -sample of \mathbf{X} (the M smallest, the M with the longest sequence of zeros in their binary representation, *etc...*).
2. A function $\hat{\xi} : [0, 1]^M \rightarrow \mathbb{R}$ which approximates θ , when applied to this M -sample.

State of the Art. Flajolet and Martin [FM85] have used these ideas to construct an algorithm based on research of patterns of 0's and 1's in the binary representation of the hashed values X_1, \dots, X_θ . It has been improved by Durand and Flajolet [DF93]. Bar-Yossef *et alii* [BYJK⁺02], have proposed 3 performant algorithms, their ideas have been generalized by Giroire [Gir05].

In a different way, Alon, Matias, and Szegedy consider estimation by *moment method*, making implementation proposed in [FM85] easier. For a nice survey about these ideas one may read [Fla04].

¹Version of January 12, 2007.

Giroire's algorithm. The starting idea in [Gir05] is to use this simple property:

$$\mathbb{E}[X_{(1)}] = \frac{1}{\theta + 1}.$$

Consequently, a naive algorithm would hash every data, compare it to the smallest hashed value already seen, and finally return $1/X_{(1)}$. Unfortunately, $\mathbb{E}[1/X_{(1)}] = \infty$. However, $1/X_{(2)}, 1/X_{(3)} \dots$ have finite expectation. This leads Giroire to propose an algorithm which return a function of $X_{(k)}$, for some k . In order to improve the precision of such an algorithm, one may wish to execute it m times with m different hashing functions, but this would cost too much time. Therefore Giroire uses *stochastic averaging*, introduced in [FM85]: the idea is to *simulate* m different experiments, by dividing $[0, 1]$ in m intervals.

Algorithm 1.

let k, m be integers. initialize $(X_{(1),i}, \dots, X_{(k),i}, i = 1, \dots, m)$ with $X_{(p),i} = \frac{i}{m}$ for all i, p .

for $j = 1$ to N

$X_j = h(Y_j)$.

let i the integer such that X_j lies in $[\frac{i-1}{m}, \frac{i}{m}[$.

update the k -dimensional vector of k smallest values $X_{(1),i}, \dots, X_{(k),i}$ lying in $[\frac{i-1}{m}, \frac{i}{m}[$.

next j .

for all p, i , renormalize $X_{(p),i} = m(X_{(p),i} - \frac{i-1}{m})$.

return an estimator $\hat{\xi} = \hat{\xi}(X_{(l),i}; i = 1, \dots, m; l = 1, \dots, k)$.

Thus we get m vectors in \mathbb{R}^k . $X_{(k),i}$ is the k -th smallest hashed value lying in $[\frac{i-1}{m}, \frac{i}{m}[$, renormalized to get a real in $[0, 1]$. If less than l values have fell in the i -th interval, then $X_{(k),i} = 1$. Obviously, Algorithm 1 makes only one pass over each data Y_i . Memory used by the algorithm is indeed M , if we have chosen $k \cdot m = M$. The estimation returned by the algorithm does not depend on any assumption on the repetitions in the sequence X_1, \dots, X_N .

Giroire [Gir05] proposes 3 estimators ξ_1, ξ_2, ξ_3 , using inverse function, square root function and log respectively. For example,

$$\xi_3 := \left(\frac{\Gamma(k-1/m)}{\Gamma(k)} \right)^{-m} \cdot e^{-\frac{1}{m} \sum_{i=1}^m \log X_{(k),i}}.$$

For each k, m these estimators are asymptotically *unbiased*, i.e. $\mathbb{E}[\xi_i] \sim \theta$ when θ goes to ∞ . Their variances are all about $1/km$. Here we give a fourth estimator, which is also asymptotically unbiased:

$$\hat{\xi} = \frac{km - 1}{\sum_{i=1}^m X_{(k),i}}.$$

Plan Using information and estimation theories, we first show that the estimator $\hat{\xi}$ is optimal under a simplified model, that we call the *independent model*. Then we discuss its actual optimality.

2 The best estimation under the *independent model*

In this section, \Rightarrow denotes the convergence in law. Recall that a real-valued random variable is said to follow the Gamma law with parameters (k, θ) if

$$\mathbb{P}(X \in [t, t + dt]) = \frac{t^{k-1}}{\Gamma(k)} \theta^k e^{-\theta t} \mathbf{1}_{t \geq 0} dt.$$

The asymptotic behavior of the minimum $X_{(1)}$ of θ random uniform variables in $[0, 1]$ is well-known (see for example [Fel70]): $X_{(1)} \Rightarrow \gamma_1$, where γ_1 follows the Gamma(1, θ) law. More generally, one can prove here the following convergence

$$(\theta X_{(k),1}, \dots, \theta X_{(k),m}) \Rightarrow [\theta \rightarrow \infty] \mathcal{L}(\gamma_1, \dots, \gamma_m), \tag{1}$$

where the γ_i are i.i.d. r.v. of law Gamma($k, 1$). Consequently, we assume in this section that the $X_{(k),i}$ are i.i.d. r.v. of law Gamma(k, θ), this is the so-called *independent model*. We set

$$\hat{\xi} = \frac{km - 1}{\sum_{i=1}^m X_{(k),i}}.$$

Remark 1. This estimator depends only on the m values $(X_{(k),i}, i = 1, \dots, m)$, not on the $km - m$ other hashed values stored by the algorithm. This follows from the fact that the knowledge of these values does not provide any information about θ . For a given i , conditionnally on $X_{(k),i}$, the r.v. $(X_{(1),i}, \dots, X_{(k-1),i})$ are distributed uniformly on $[0, X_{(k),i}]$.

A simple calculation shows that under the independent model,

$$\begin{aligned}\mathbb{E}[\hat{\theta}] &= \theta, \\ \text{Var}(\hat{\theta}) &= \frac{\theta^2}{km - 2}.\end{aligned}$$

This is indeed better than the 3 estimators proposed in [Gir05].

Recall a few definitions in Statistics (see for example [Leh83]): given a m -sample of i.i.d. random variables X_1, \dots, X_m of some law P_θ , any random variable $S = S(X_1, \dots, X_m)$ is called a *statistic*. Here we consider the statistic $S = \sum_{i=1}^m X_{(k),i}$.

Definition 1. A statistic S is sufficient for the parameter θ if and only if, conditionnally to S , the law of (X_1, \dots, X_m) does not depend on θ .

More informally, S is sufficient if, given S , the knowledge of (X_1, \dots, X_m) does not give any information on θ . \hat{S} is sufficient.

Definition 2. A statistic S is complete if whenever $h(S)$ is a function of S for which $\mathbb{E}[h(T)] = 0$ for all θ , then $h \equiv 0$, P_θ almost everywhere.

Here, the statistic $S = \sum_{i=1}^m X_{(k),i}$ is complete and sufficient. Some simple criterions to check sufficientness and completeness are given in [Leh83]. Complete sufficient statistics share the following useful property:

Theorem 1 (Lehmann-Scheffé). Let S be a sufficient and complete statistic. Let ξ^* be another unbiased (i.e. $\mathbb{E}[\tilde{\xi}] = \theta$) estimator of θ . Among all the unbiased estimators of θ , $\mathbb{E}[\xi^*|S]$ has a minimal variance. Such an estimator is said to be efficient.

Corollary 1. Let $\tilde{\xi}$ another unbiased estimator of θ . Under the independent model,

$$\mathbb{E}[(\tilde{\xi} - \theta)^2] \geq \mathbb{E}[(\hat{\xi} - \theta)^2].$$

Remark 2. Note that $\text{Var}(\hat{\xi})$ is about θ^2 . This optimal bound does not depend on the algorithm, see [PD03].

3 Optimality in the real model

From now one places oneself in the *exact model*: $X_{(p),i}$ is the p -th smallest realization of θ i.i.d. r.v. uniform on $[0, 1]$, among the values lying in $[\frac{i-1}{m}, \frac{i}{m}]$. When $i \neq j$, there is now dependency between $X_{(k),i}$ and $X_{(k),j}$. Set \mathbf{P} and \mathbf{P}_{ind} the laws corresponding respectively to the exact and independant models, \mathbb{E} and \mathbb{E}_{ind} the corresponding expectations.

Lemma 1. Let A be the event

$$A = A_{k,m,\theta} : \text{“for all } i = 1, \dots, m, X_{(k),i} < \frac{1}{m}\text{”}.$$

(i.e. at least k hashed values have fallen in each of the m intervals). From a classical inequality (see [Bol85]) we get

$$\mathbf{P}(A) \geq 1 - 2me^{-\frac{\theta}{2m^2}}.$$

Here is the main result:

Theorem 2 (Optimality in the exact model). Let $\tilde{\xi}(\mathbf{X})$, with $\mathbf{X} = (X_1, \dots, X_m)$ another estimator of θ . Let $b(\theta)$ be the bias $\mathbb{E}_\theta[\tilde{\theta} - \theta]$. We assume

1. $b(\theta) = O(\sqrt{\theta})$.
2. There exists a constant C such that $|\tilde{\xi}(\mathbf{x})| \leq \frac{C}{\|\mathbf{x}\|}$, for every \mathbf{x} in \mathbb{R}^m , $\|\mathbf{x}\|$ large enough.

Then

$$\mathbb{E}_\theta[(\tilde{\theta} - \theta)^2] \geq \mathbb{E}_\theta[(\hat{\theta} - \theta)^2] + O(\theta).$$

Proof. First write

$$\begin{aligned} \mathbb{E}[(\tilde{\theta} - \theta)^2] &= \mathbb{E}[(\tilde{\theta} - \theta)^2 \mathbf{1}_A] + \mathbb{E}[(\tilde{\theta} - \theta)^2 (1 - \mathbf{1}_A)], \\ &= \mathbb{E}[(\tilde{\theta} - \theta)^2 \mathbf{1}_A] + o(\theta), \end{aligned}$$

using Lemma 1. We now bring back ourselves to the independant model:

$$\mathbb{E}[(\tilde{\theta} - \theta)^2] = \mathbb{E}_{\text{indé}}[(\tilde{\theta} - \theta)^2] + (\mathbb{E}[(\tilde{\theta} - \theta)^2 \mathbf{1}_A] - \mathbb{E}_{\text{indé}}[(\tilde{\theta} - \theta)^2]) + o(A), \quad (2)$$

The key point is the fact that conditioned to the event A , the r.v. $(X_{(k),1}, \dots, X_{(k),m})$ admit a density toward the Lebesgue measure on \mathbb{R}_+ .

$$\begin{aligned} \mathbb{E}[(\tilde{\theta} - \theta)^2] - \mathbb{E}_{\text{indé}}[(\tilde{\theta} - \theta)^2] &= \\ &= \int_{[0, \frac{1}{m}]^m} \binom{\theta}{(k-1) \dots (k-1) \ 1 \dots 1} x_1^{k-1} \dots x_m^{k-1} (1 - x_1 - \dots - x_m)^{\theta - mk} dx_1 \dots dx_m \\ &\quad - \int_{\mathbb{R}_+^m} \frac{x_1^{k-1}}{\Gamma(k)} \dots \frac{x_m^{k-1}}{\Gamma(k)} \theta^{km} e^{-\theta(x_1 + \dots + x_m)} dx_1 \dots dx_m. \end{aligned}$$

We omit the proof of the following lemma:

Lemma 2.

$$\left| \frac{\theta(\theta-1)\dots(\theta-2k+1)}{\theta^{2k}} (1 - x_1 - \dots - x_m)^{\theta-2k} - e^{-\theta(x_1 + \dots + x_m)} \right| \leq c^{ste} \theta (x_1 + \dots + x_m)^2 e^{-\theta(x_1 + \dots + x_m)},$$

where the constant depends neither on θ nor on the x_i 's.

Hence

$$\begin{aligned} |\mathbb{E}[(\tilde{\theta} - \theta)^2] - \mathbb{E}_{\text{indé}}[(\tilde{\theta} - \theta)^2]| &\leq \\ &\leq \int_{[0, \frac{1}{m}]^m} |\tilde{\theta}(x_1, \dots, x_m) - \theta|^2 \frac{x_1^{k-1}}{\Gamma(k)} \dots \frac{x_m^{k-1}}{\Gamma(k)} \theta^{km} \left\{ c^{ste} \theta (x_1 + \dots + x_m)^2 e^{-\theta(x_1 + \dots + x_m)} \right\} dx_1 \dots dx_m + O(\theta) \end{aligned}$$

Set $y_i = \theta x_i$, $i = 1 \dots m$ in the integrand:

$$\leq \int_{[0, \frac{\theta}{m}]^m} \left| \tilde{\theta}\left(\frac{y_1}{\theta}, \dots, \frac{y_m}{\theta}\right) - \theta \right|^2 \frac{x_1^{k-1}}{\Gamma(k)} \dots \frac{x_m^{k-1}}{\Gamma(k)} \theta^{-1} \left\{ c^{ste} \theta (y_1 + \dots + y_m)^2 e^{-\theta(y_1 + \dots + y_m)} \right\} dy_1 \dots dy_m + O(\theta)$$

Here we use the hypothesis made on the estimator: $\theta(\mathbf{x}) \leq \frac{1}{\|\mathbf{x}\|}$. We also need the following arithmetico-geometric inequality:

$$(a_1 \dots a_m)^\alpha \leq \lambda (a_1^2 + \dots + a_m^2)^{m\alpha/2}.$$

Set $\mathbf{y} = (y_1, \dots, y_m)$, one gets

$$\begin{aligned} &\leq c^{ste} \int_{[0, \frac{\theta}{m}]^m} \frac{\theta^2}{\|\mathbf{y}\|^2} (\|\mathbf{y}\|)^{m(k-1)} \theta^{-1} (y_1 + \dots + y_m)^2 e^{-y_1 - \dots - y_m} dy_1 \dots dy_m + O(\theta) \\ &\leq c^{ste} \int_{[0, \frac{\theta}{m}]^m} \frac{\theta^2}{\|\mathbf{y}\|^2} (\|\mathbf{y}\|)^{m(k-1)} \theta^{-1} (\|\mathbf{y}\|)^2 e^{-\|\mathbf{y}\|} dy_1 \dots dy_m + O(\theta). \end{aligned}$$

Here we make a ‘‘polar-like’’ change of variables in \mathbb{R}^m . We get this inequality:

$$\begin{aligned} |\mathbb{E}[(\tilde{\theta} - \theta)^2] - \mathbb{E}_{\text{indé}}[(\tilde{\theta} - \theta)^2]| &\leq c^{ste} \theta \int_0^{\sqrt{m} \frac{\theta}{m}} r^\alpha e^{-r} dr + O(\theta), \quad \alpha > 0. \\ &= O(\theta). \end{aligned}$$

(2) has become

$$\begin{aligned}\mathbb{E}[(\tilde{\theta} - \theta)^2] &= \mathbb{E}_{\text{indé}}[(\tilde{\theta} - \theta)^2] + O(\theta) \\ &= \mathbb{E}_{\text{indé}}[(\hat{\theta} - b(\theta) - \theta)^2] + b^2(\theta) + O(\theta) \\ &\geq \mathbb{E}_{\text{indé}}[(\hat{\theta} - \theta)^2] + O(\theta),\end{aligned}$$

□

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