# Analyzing statistical and computational tradeoffs of estimation procedures \*

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#### Abstract

The recent explosion in the amount and dimensionality of data has exacerbated the need of trading off computational and statistical efficiency carefully, so that inference is both tractable and meaningful. We propose a framework that provides an explicit opportunity for practitioners to specify how much statistical risk they are willing to accept for a given computational cost, and leads to a theoretical risk-computation frontier for any given inference problem. We illustrate the tradeoff between risk and computation and illustrate the frontier in three distinct settings. First, we derive analytic forms for the risk of estimating parameters in the classical setting of estimating the mean and variance for normally distributed data and for the more general setting of parameters of an exponential family. The second example concentrates on computationally constrained Hodges-Lehmann estimators. We conclude with an evaluation of risk associated with early termination of iterative matrix inversion algorithms in the context of linear regression.

Keywords: Risk; Computation; Exponential Family.

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#### 1 Introduction

The advent of massive datasets in applied fields has been heralded as a new age for statistics but these datasets are both a blessing and a curse. They offer the opportunity to improve the precision and efficiency of statistical methods but frequently these improvements come at high computational costs. Up until recently, the computational aspects of statistics had been largely ignored by the statistics literature with those concerns relegated to other fields. Statisticians have begun to explore computationally more efficient techniques for disparate problems using ideas like variational methods (Wainwright and Jordan, 2008), parallel MCMC (Scott et al, 2013), stochastic gradient descent (Langford et al, 2009; Bottou, 2012; Agarwal et al, 2014; Toulis and Airoldi, 2014), and convex relaxations (Chandrasekaran and Jordan, 2013).

Recent efforts have begun to evaluate the computational cost of many statistical procedures and conversely the statistical risk of computationally efficient procedures while introducing new procedures that balance these ideas. Kleiner et al (2014) describes a procedure known as the "bag of little bootstraps," a data splitting technique that allows for computationally tractable implementation of the bootstrap for massive datasets. Wang et al (2014) study the classical problem of covariance estimation under computational constraints. Yang et al (2015) find conditions that ensure a Markov chain Monte Carlo sampler for Bayesian linear regression in high dimensions will be both consistent and have fast mixing time. Chandrasekaran and Jordan (2013) consider "algorithm weakening" to describe an ordering of algorithms in terms of compute time and statistical properties. Horev et al (2015) study the tradeoff between statistical detection and computation in an edget detection framework.

A common approach is to describe compute cost in terms of algorithmic complexity (Berthet and Rigollet, 2013; Shender and Lafferty, 2013; Bresler et al, 2014; Montanari, 2014). Within this framework, two algorithms are equivalent if they have the same worst

case complexity, even if one of them is likely to never perform in the worst case regime. While computational complexity is a key aspect of understanding and choosing between algorithms, when a finer analysis is possible, it is preferred. Chandrasekaran and Jordan (2013) provides an example of this finer analysis via the "time-data tradeoff" and our approach is in a similar spirit. Specifically, we consider a practical framework for addressing the tradeoff between computational cost and statistical risk. This is in contrast to other works such as Montanari (2014), who shows that some statistical procedures can be modified to provide fast algorithms with well understood computational gains but without assessing the degradation in statistical risk.

Our focus for this paper will be on classical statistical problems including estimating the mean and variance for a normal population, exponential families, robustness, and regression. In Section 2, of this paper we outline the basic framework associated with the statistical risk and computational cost tradeoff frontier. Section 3 illustrates this framework in the normal population setting and in Section 4 we extend these ideas to general exponential families. We briefly consider robust estimates such as the Hodges-Lehmann example in Section 5. Finally, we consider extending these ideas to iterative methods for matrix inversion in Section 6.

### 2 Analyzing statistical and computational tradeoffs

Consider the problem of estimating  $\theta$  given an i.i.d. sample from the distribution  $f_{\theta}$ . We suppose that the parameter is vector valued with  $\theta \in \Theta \subset \mathbb{R}^p$ , the model is  $\{f_{\theta} : \theta \in \Theta\}$  and we denote our random sample as  $X_1, \ldots, X_n \stackrel{iid}{\sim} f_{\theta}$  where  $X_i$  is  $\mathcal{X}$  valued for  $\mathcal{X} \subset \mathbb{R}^d$ . The estimate is denoted is  $\hat{\theta} = \hat{\theta}(X_1, \ldots, X_n)$  and the loss associated with the estimate is  $\ell(\hat{\theta}, \theta)$ . In classical statistical estimation theory, one seeks to in some way minimize the risk, the expected loss  $R(\hat{\theta}, \theta) = \mathbb{E}_{\theta}[\ell(\hat{\theta}, \theta)]$ , be it in terms of minimax optimality, Bayesian optimality, or other principles such as unbiasedness or equivariance (Lehmann and Casella, 1998).

We will maintain the goal of achieving a small risk but we will add the goal of computing the estimate quickly. Formally, one need not have an algorithm to compute the estimator  $\hat{\theta}: \mathcal{X}^n \mapsto \Theta$  for all values in  $\mathcal{X}^n$  in order to analyze the risk and statistical properties of the estimate. However, in our setting we will assume that each estimator comes equipped with an algorithm to compute the function of the data. Hence, an estimate, together with its algorithm, will have a compute time  $C(\hat{\theta}) \in \mathbb{R}^+$  that denotes the runtime of that algorithm on the data  $X_1, \ldots, X_n$ . Altogether we now have two quantities, the risk  $R(\hat{\theta}, \theta)$  and the expected compute time  $\mathbb{E}_{\theta}[C(\hat{\theta})]$ .

**Remark.** To keep things more straightforward, the first few examples considered in this manuscript will have the property that  $C(\hat{\theta})$  does not depend on the data  $X_1, \ldots, X_n$  so that the expected compute time does not depend on the parameter. Clearly many algorithms do not fit this mold and much of the ideas we discuss apply outside the fixed computational cost setting.

Now, consider a practitioner confronted with a collection of estimators, each with an associated algorithm. We denote this collection by  $\{\hat{\theta}_s\}_{s\in S}$  where S is some index set. The collection of estimates may be determined by questions such as: How much storage is available? Can all the data be kept in memory or only a subset? How much processing power is available? Are there parallel or distributed systems that can be exploited?

Each of these questions will put different constraints on the collection of estimators that delineates what is possible and ready for use. Among the feasible estimators, the practitioner must chose an estimator  $\hat{\theta}_s$  to use on the data at hand. If the practitioner knows  $R(\hat{\theta}_s, \theta)$  and  $C(\hat{\theta}_s)$  for each estimate and parameter value than they can use this to make an informed decision about which estimator to choose that balances risk and computational cost. For a given parameter value  $\theta$  we can plot the risk and computation time associated with each estimator as was done in Figure 1. This figure illustrates the idea of a computational-statistical trade-off with some estimates achieving very low risk, others being very fast,

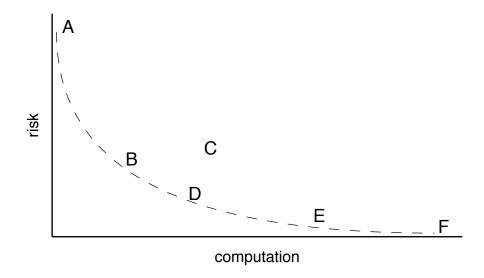


Figure 1: An illustration the risk and computation time trade-off associated with a collection of 6 estimators. Estimator A is the fastest estimators but has much higher risk than the other estimators while estimator F has the lowest risk but suffers from being quite slow. Estimators B or D might be a good choice for a practitioner seeking to achieve a balance between time and accuracy. Note that estimator C can be disregarded since both B and D are strictly better than C in terms of both risk and computation time. The dashed line depicts the theoretical risk-computation frontier.

and some providing a balance between the two. In the next section we will examine this framework in the setting estimating the mean and variance for a sample from a normal distribution before investigating exponential families in general in Section 4.

#### 3 Normal example

To concretely illustrate the computation-statistical tradeoffs we will consider the simple example of estimating the population mean and variance from a sample of independent and identically distributed normal random variables. We consider two computational constraints that define the collections of algorithms that are available for estimation. The first setting explores a singly indexed set of estimators for a near zero resource streaming setting. The second setting generalizes the first by allowing various ways to divide the data between

different aspects of the estimation.

#### 3.1 Standard inference

Suppose that we observe  $X_1, \ldots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$  and we want to estimate  $\theta = (\mu, \sigma^2)$  with our loss being square error loss,  $\ell(\hat{\theta}, \theta) = \|\hat{\theta} - \theta\|_2^2 = (\hat{\mu} - \mu)^2 + (\hat{\sigma}^2 - \sigma^2)^2$ . Our analysis allows for loss functions that are other linear combinations of the risks for  $\mu$  and  $\sigma^2$  however for ease of illustration we focus on this loss function.

Before delving into various computationally constrained estimates, consider the standard maximum likelihood estimates (MLE) of the mean and variance for a normal.

$$\hat{\mu}_{\text{MLE}} = \overline{X} = \frac{1}{n} \sum_{i=1}^{n} X_i \quad \text{and} \quad \hat{\sigma}_{\text{MLE}}^2 = \overline{X}^2 - \overline{X}^2 = \frac{1}{n} \sum_{i=1}^{n} X_i^2 - \overline{X}^2. \tag{1}$$

To compute this estimate we require two operations or looks at each data point to compute the sufficient statistics  $\overline{X}$  and  $\overline{X^2}$ —that is we need to temporarily store each data point in order to perform a local operation before updating the sufficient statistics. This paradigm of "looking" at data point and performing an operation with them defines our computation cost in this problem. The total computational cost for the MLE is thus 2n. The risk associated with this estimate is

$$\mathbb{E}\left[(\hat{\mu}_{MLE} - \mu)^2\right] + \mathbb{E}\left[(\hat{\sigma}_{MLE}^2 - \sigma^2)^2\right] = \frac{\sigma^2}{n} + \frac{2\sigma^4}{n}.$$

#### 3.2 Streaming setting

We now consider what we call the streaming setting, a near zero-resource setting where local storage is extremely limited, allowing us access to each data point exactly once. This means

One might claim the cost is 2n + C where the C represents the additional computation needed to complete the computations in Eq. (1). We omit this since this additional time is unchanged for all estimates and algorithms in this section.

that we can't compute the full MLE which requires two looks at each point to compute the first and second moments. We consider estimators with index set  $S = \{1, ..., n-1\}$  where for each  $s \in S$  the estimate  $\hat{\theta}_s$  is computed by first computing the moment sums

$$M_{1,s} = \sum_{i=1}^{s} X_i, \quad M_{2,s} = \sum_{i=s+1}^{n} X_i^2,$$

where n is the total sample size. We could have allowed the sums to be non-sequential but provided s samples are used for  $M_{1,s}$  and n-s for  $M_{2,s}$  the estimates are the same in risk and computation time due to the fact that the samples are exchangeable. We assume that updating either  $M_{1,s}$  or  $M_{2,s}$  has the same cost so that the cost of computing these statistics is exactly n as each data point is accessed only once and again we can simply keep track of two sufficient statistics.

Remark. We remark here that assigning a cost of n to each of these estimators is, of course, an abstraction but a useful one nonetheless. In reality the time to compute an estimate will be some function of n, s, and will also depend on the implementation in high-level and low-level languages down to the structure of the hardware being used. However, for a large range of n and s we believe it is reasonable to assume that the cost to compute  $M_{1,s}$  and  $M_{2,s}$  will be linear in s and n-s respectively. Boiling this down to the assumption that the cost is n makes the following analysis quite clear but generalizing slightly does not change the overall flavor of the result as we discuss at the end of Section 4. As we go forward, this paper we will make similar assumptions about the computational cost that allow for numerical analysis but do not impact the overall framework.

From these statistics we can define the unbiased streaming estimates for the mean and

variance as as

$$\hat{\mu}_s = \frac{1}{s} M_{1,s}$$
, and 
$$\hat{\sigma}_s^2 = \frac{s}{(s-1)(n-s)} \left( M_{2,s} - \frac{n-s}{s} M_{1,s}^2 \right).$$

We note that unlike in the example of the MLE where estimates of the mean and the variance are independent, for the streaming setting the estimates of the mean and the second non-central moment are independent while the estimates of the mean and the variance are not. This will be explored in greater detail in Section 4 when discussing estimates of natural versus mean value parameters for general exponential families.

The risks of the mean and variance, both under quadratic loss, in the streaming setting are given by

$$R(\hat{\mu}_s, \mu) = \frac{\sigma^2}{s}$$

$$R(\hat{\sigma}_s^2, \sigma^2) = \frac{2sn\mu^2\sigma^2 + 2((s-1)s + n)\sigma^4}{(s-1)^2(n-s)}.$$

Alternatively, we could consider the maximum likelihood estimate given the observed statistics  $M_{1,s}$ ,  $M_{2,s}$  and t:

$$\hat{\mu}_{MLE,s} = \frac{1}{s} M_{1,s} \text{ and } \hat{\sigma}_{MLE,s}^2 = \frac{1}{n-s} M_{2,s} - \left(\frac{1}{t} M_{1,s}\right)^2.$$
 (2)

As n gets larges and t/n tends to a constant  $p \in (0,1)$ , these estimates are essentially equivalent and will both have the same asymptotic risk. Indeed, asymptotically we have that the risk is approximately

$$\frac{\sigma^2 (4\mu^2 + 2p\sigma^2 - p + 1)}{np(1-p)}$$

and one can then verify that in order to minimize this asymptotic risk as a function of  $(\mu, \sigma)$  one should select  $p = \frac{\sqrt{4\mu^2+1}}{\sqrt{4\mu^2+2\sigma^2}+\sqrt{4\mu^2+1}}$ . Intuitively, this says that if the signal to noise ratio is very small, than p is close to zero with most effort put on computing the second moment  $M_{2,s}$ . On the other hand if  $\sigma^2 \ll \mu^2$  and  $\mu \gg 0$  then p will be close 1/2. Finally, if  $\sigma^2 \ll \mu^2$  and  $\mu \approx 0$  then p will be close to 0.

#### 3.3 Risk/computation frontier

The streaming setting is a special case of a slightly more general collection of estimators. In particular, we allow up to two looks and operations for each point with some points possibly only used for the computation of one of the two statistic, others may be used for both, while still other samples may be ignored completely. The collection of estimates is indexed by pairs of sets  $(S_1, S_2)$  where each  $S_i$  is a non-empty subset of  $\{1, \ldots, n\}$  so the index set is

$$S = \{ (S_1, S_2) : S_1 \subset [n], |S_2 \subset [n], |S_1| > 0, |S_2| > 0 \}.$$
(3)

For  $s = (S_1, S_2) \in S$  we first compute

$$M_{1,s} = \sum_{i \in S_1} X_i, \quad M_{2,s} = \sum_{i \in S_2} X_i^2,$$
 (4)

and we let  $n_1 = |S_1 \setminus S_2|$ ,  $n_2 = |S_2 \setminus S_1|$  and  $n_{12} = |S_1 \cap S_2|$ . As in the previous setting, the particular sets  $S_1$  and  $S_2$  only impact the risk and computation time of the estimates in terms of  $n_1$ ,  $n_2$  and  $n_{12}$ . The computational cost we assign to this procedure is

$$C = n_1 + n_2 + 2n_{12}$$

since  $n_{12}$  indicates the number of samples used for both statistics while  $n_1$  and  $n_2$  indicate the number of samples used only for computing  $M_{1,s}$  and  $M_{2,s}$ , respectively. Our maximum-

likelihood-like estimates are then

$$\hat{\mu}_s = \frac{1}{n_1 + n_{12}} M_{1,s} \text{ and } \hat{\sigma}_s^2 = \frac{1}{n_2 + n_{12}} M_{2,s} - \hat{\mu}_s^2$$

To get the risk of these estimators we provide a glimpse of the general Fisher information result from the following section.

**Proposition 1.** Let  $X_1, \ldots, X_n \sim \text{normal}(\mu, \sigma^2)$ . For  $s = (S_1, S_2) \in S$  from Eq. (3), let  $M_{1,s}$ ,  $M_{2,s}$ ,  $n_1$ ,  $n_2$  and  $n_{12}$  be as in Eq. (4). For n large, the covariance for estimates  $(\hat{\mu}_s, \hat{\sigma}_s^2)$  of  $(\mu, \sigma)$  is approximately

$$\begin{pmatrix}
\frac{\sigma^2}{n_1 + n_{12}} & -\frac{2n_2\mu\sigma^2}{(n_1 + n_{12})(n_{12} + n_2)} \\
-\frac{2n_2\mu\sigma^2}{(n_1 + n_{12})(n_{12} + n_2)} & \frac{2(n_1 + n_{12})\sigma^4 + 4(n_1 + n_2)\mu^2\sigma^2}{(n_1 + n_{12})(n_{12} + n_2)}
\end{pmatrix}$$
(5)

and so the overall risk of the estimates is approximately

$$\frac{\sigma^2}{n_1 + n_{12}} + \frac{2(n_1 + n_{12})\sigma^4 + 4(n_1 + n_2)\mu^2\sigma^2}{(n_1 + n_{12})(n_{12} + n_2)}.$$

For a given  $\mu$  and  $\sigma$  we can compute  $n_1$ ,  $n_2$  and  $n_{12}$  that minimize the total risk for any given computational cost C satisfying  $2 \le C \le 2n$ . Several scenario, in terms of the signal

SNR	$\sigma^2$	$n_1/n$	$n_2/n$	$n_{12}/n$	
=0	> 1/2	2 Change points			
=0	= 1/2	Non-unique Solution			
=0	< 1/2	2 Change points			
$\geq 1$	> 0	0	0	C/2	
$\in (0,1)$	> 1/2	0	$a_C$	$\overline{(C-a_C)/2}$	
$\in (0,1)$	= 1/2	0	0	C/2	
$\in (0,1)$	< 1/2	$b_C$	0	$(C-b_C)/2$	

Table 1: The split of the data points between the three possible usages (mean only, non central second moment only, or both) is provided in columns 3 through 5. Both  $a_C$  and  $b_C$  approach to 0 as  $C \to 2n$ . See Figure 1 for a detailed look at particular parameter values in these different regimes.

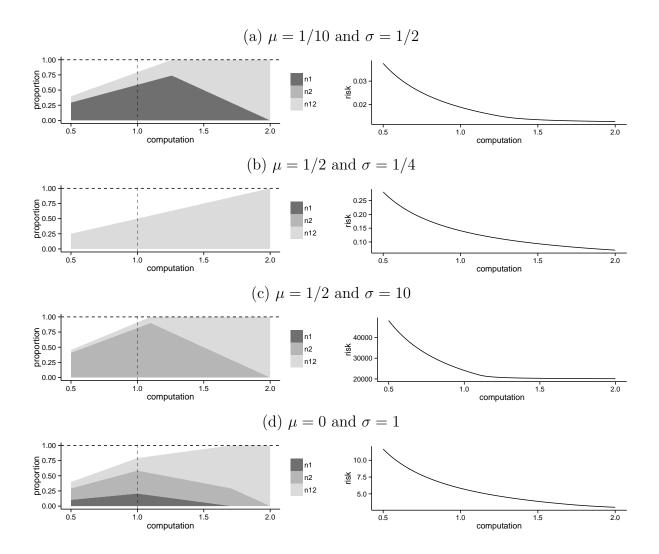


Figure 2: In each row, the left panel illustrates the optimal proportions  $n_1/n$  in red,  $n_2/n$  in green and  $n_{12}/n$  in blue as a function of the computational constraints given along the horizontal axis. The computational constraint is given as a proportion of the number of samples n, so that on the horizontal axis 1 indicates a cost of n and 2 indicates a cost of 2n, where the standard estimate is always optimal. The right panel illustrates the risk using the given estimate with the given proportions. Each of the rows corresponds to a different row in Table 3.3.

to noise ratio SNR =  $\mu/\sigma$  and variance  $\sigma$  are presented in Table 3.3. In particular, we note that if SNR =  $1/\sqrt{2}$  we always choose to use less of the data and essentially construct an MLE. Otherwise, there are different optimal  $n_1$ ,  $n_2$  and  $n_{12}$  based on whether SNR is zero or between 0 and 1 and on whether  $\sigma^2$  is greater than, equal to, or less than 1/2. To further illustrate the different regimes, Figure 2 shows the optimal portions of the samples used and

the associated risk as the computational constraint varies. In the next section we explore the tradeoff of risk and compute time for the more general setting of exponential families.

## 4 Exponential family

A p parameter exponential family is a family of distributions  $\{f_{\theta}\}_{{\theta}\in\Theta}$  on a space  $\mathcal{X}$  each with a density with respect to an appropriate carrying measure  $\mu$  which can be written in the form

$$f_{\theta}(x) = h(x) \exp\{\theta^T t(x) - \Psi(\theta)\}$$

where h is a function from  $\mathcal{X}$  to  $\mathbb{R}^+$ ,  $\theta \in \Theta \subset \mathbb{R}^p$  is the natural parameter for the model,  $t = (t_1, t_2, \dots, t_p)^t$  is a real-valued p-dimensional sufficient statistic, ie.  $t_k : \mathcal{X} \mapsto \mathbb{R}$ , and  $\Psi(\theta) = \log \int_{\mathcal{X}} h(x) \exp\{\theta^T T(x)\} dx$ , (Bickel and Doksum, 1976).

For a random sample  $X_1, \ldots, X_n \stackrel{iid}{\sim} f_{\theta}$ , the statistic  $T = \sum_{i=1}^n t(X_i) \in \mathbb{R}^p$  is sufficient and the maximum likelihood estimate  $\theta$  is found by solving for  $\theta$  in the equation  $T/n = \mathbb{E}_{\theta}[t(X)]$ . As in the normal example, for our purposes it is convenient to reparameterize the model using the mean value parameterization with parameters  $\tau = \tau(\theta) = \mathbb{E}_{\theta}[T(X)] \in \mathbb{R}^p$  where the MLE for  $\tau$  is simply T/n. Note that the map  $\tau : \theta \to \tau(\theta)$  is invertible so that  $\tau$  is a proper reparametrization of the model.

Using the same ideas as in our normal example, we can construct alternative statistics by computing each component of the sufficient statistic on a subset of the full data set. Formally, our estimates will be indexed by subsets  $S_1, \ldots, S_p \subset [n]$  so the index set is  $\mathcal{S} = (2^{[n]})^p$ . For  $S = (S_1, \ldots, S_p) \in \mathcal{S}$ , we define the statistics

$$T_S = \left(\sum_{i \in S_1} t_1(X_i), \dots, \sum_{i \in S_p} t_p(X_i)\right)$$

 $<sup>^{2}</sup>$ Again, the actual sets are not critical but only their cardinality and the cardinality of the pairwise interections.

and the estimate for  $\tau_k$  is  $\hat{\tau}_{S,k} = |S_k|^{-1} T_{S,k}$ . The estimate for  $\theta$  is defined analogously,  $\hat{\theta}_S = \tau^{-1}(\hat{\tau}_S)$ .

The covariance for  $\hat{\tau}_S$  can be written in terms of the covarariance for T(X) which is  $I^{-1}(\tau)$ , the inverse of the Fisher information matrix for  $\tau$ , and the cardinality of the sets  $S_1, \ldots, S_p$  and their pairwise intersections. Specifically, the variance terms are  $\text{Var}(|S_k|^{-1}T_{S,k}) = \frac{I^{-1}(\tau)_{kk}}{|S_k|^2}$  and the covariance terms are  $\text{Cov}(|S_k|^{-1}T_{S,k}, |S_l|^{-1}T_{S,l}) = \frac{|S_k \cap S_l|I^{-1}(\tau)_{kl}}{|S_k| \cdot |S_l|}$ .

Note that the analog to the streaming case for a p-parameter exponential family is where  $S_k \cap S_l = \emptyset$  for all  $k \neq l \in [p]$  and in this case the covariance matrix for  $\hat{\tau}_S$  will be diagonal as is evident by the fact that each statistic is computed on an independent sample. However the covariance for  $\hat{\theta}_S$  will usually not be diagonal, as can be verified in the case of the normal example.

For a given cost level c and estimate  $\theta = \theta(\tau) = \tau^{-1}(\tau)$  we can find the best subsets by solving an appropriate optimization problem. Frequently the compute times for each statistic will be different and so we can define the computational cost for each statistic in terms of the cost to compute  $t_k(x)$  and the set sizes  $|S_k|$  for  $k \in [p]$ . Specifically, we denote by  $c_k$  the runtime to perform the operation that computes  $t_k(x_i)$  and adds it to the partial sum. The risk for estimating  $\theta$  is  $R(\theta, \hat{\theta}_S) = \operatorname{tr}\left(\dot{\theta}(\tau)\operatorname{Cov}(\hat{\tau}_S)\dot{\theta}(\tau)^T\right)$  but if we want to estimate another parameter  $\eta = \eta(\tau)$  then the risk is given by  $\operatorname{tr}(\dot{\eta}(\tau)\operatorname{Cov}(\hat{\tau}_S)\dot{\eta}(\tau)^T)$  where  $\dot{\eta}(\tau)$  is the gradient of  $\eta$  with respect to  $\tau$ . Finally, some parameters may be more important to estimate than others and so we allow for the scaling of the covariance by a non-negative diagonal matrix Q which indicates the relative importance of the different components of

the parameter. Together this yields the optimization problem

$$\min_{S \in \mathcal{S}} \quad R(\eta, \hat{\eta}_S) = \operatorname{tr}(Q\dot{\eta}(\tau)\Sigma\dot{\eta}(\tau)^T) \tag{6}$$

$$\min_{S \in \mathcal{S}} R(\eta, \hat{\eta}_S) = \operatorname{tr}(Q\dot{\eta}(\tau)\Sigma\dot{\eta}(\tau)^T)$$
such that
$$\sum_{k=1}^{p} c_k |S_k| \le c,$$
(7)

where 
$$\Sigma_{kl} = \begin{cases} \frac{I^{-1}(\tau)_{kk}}{|S_k|^2}, & \text{if } k = l\\ \frac{|S_k \cap S_l|I^{-1}(\tau)_{kl}}{|S_k| \cdot |S_l|} & \text{otherwise.} \end{cases}$$
 (8)

In Section 3 we were able to solve this problem in the case of the normal distribution and estimation of the mean and variance parameters. Solving this problem for certain other distributions such as the multivariate normal is also relatively straightforward. In general, computing the Fisher information matrix and its inverse for the mean value parameterization of an exponential family is a nontrivial task. Additionally, the functions  $\eta(\tau)$  are generally difficult to compute especially in high dimensions. For example, Montanari (2014) shows that for certain classes of graphical models finding computing the map from the mean-value to the natural parameter space is an NP-hard problem in the dimension of the parameter space. Nonetheless, the formulation of this optimization problem offers another step towards an understading the frontier of the risk-runtime tradeoff. In the next two sections we will deviate slightly and consider estimation procedures with slightly less well understood

#### Hodges-Lehmann estimator 5

As another investigation into possible tradeoffs between computation time and statistical risk we consider the Hodges-Lehmann (HL) estimate for the mean of a distribution. For a sample of size n, this estimates is defined as

$$\hat{\theta}_{HL} = \operatorname{median}\left\{\frac{X_i + X_j}{2} : i, j \in [n]\right\}. \tag{9}$$

This estimate is known to be very robust and often outperforms both the mean and the median in terms of statistical risk for data arising from distributions with contamination. In this example we consider the contaminated distribution

$$(1-\alpha)\mathcal{N}(0,1) + \alpha\mathcal{T}_3(4)$$

where  $\mathcal{T}_3(4)$  is a central t distribution with three degrees of freedom and then scaled by a factor of four. Each mixture component has mean zero however approximately ten percent of any sample will be from a contaminated distribution with much heavier tails and higher variance. The proportion of data arising from the t distribution is the contamination level  $\alpha$ .

The computation cost of HL estimator can be decomposed into two parts, the time to compute the pairwise sums, which requires n(n+1) looks at the data, and the time to compute the median. The time to compute the median is dominated by the number of comparisons needs and will in practice depend on the data. For the simulations below we add the the expected number of comparisons, as determined in Knuth (1972) for the QuickSelect algorithm, to the computation cost. Asymptotically, the expected time to compute the median of n samples is approximately 3.38n, while in comparison, the mean requires only n operations as described above. We considered a variety of estimates in order to reduce the computation time of the HL estimate and compare them in Figure 3:

**subset** We first select a subset of the data of m and then sample without replacement c/2 from all  $\binom{m}{2}$  pairs in this subset.

**sample** We sample with replacement c/2 pairs from all  $\binom{n}{2}$  possible pairs from the entire

data set.

**sequential** At cost c we use the c/2 pairs  $(X_1, X_2), (X_3, X_4), \dots, (X_{c-1}, X_c)$ 

For each of these estimates we compute the mean for each of the selected pairs and then compute the median for that set.

We used a sample size of n = 2000 and for the subset HL estimate we used  $m = \lfloor \sqrt{2000} \rfloor$ . For the mean we simply considered the sample mean of the first c points for  $c \in [n]$  and for the three HL estimates we used even costs from 2 to n. We simulated  $5 \times 10^4$  replicates for each contamination level to estimate the risk associated with each estimator at each cost. Overall, the best estimates were either the sample mean or the sequential HL, at least up to the feasible costs for those methods. Choosing between the sample mean and the HL sequential depends on the cost restraints as well as the contamination level as shown in Figure 3. Overall, this example illustrates the intricacies of the computational-statistical trade-off frontier for even relatively straightforward settings.

#### 6 Matrix inversion

One of the most important linear algebra operations for statistical analysis is the matrix inverse. It is also frequently the bottleneck of statistical procedures as the operation is naively of complexity order  $\mathcal{O}(n^3)$  (Gauss-Jordan elimination) and optimally, if impractically, of order  $\mathcal{O}(n^{2.373})$  (Williams, 2012). All practical algorithms for matrix inversion are based on iterative approaches. Each iteration can naturally define a computational cost metric that allows us to evaluate the statistical risk versus computational cost tradeoff within an algorithm. Since all iterative methods are meant to converge to the same numerical value this also suggests a method for comparing across algorithms when explicit costs cannot be defined.

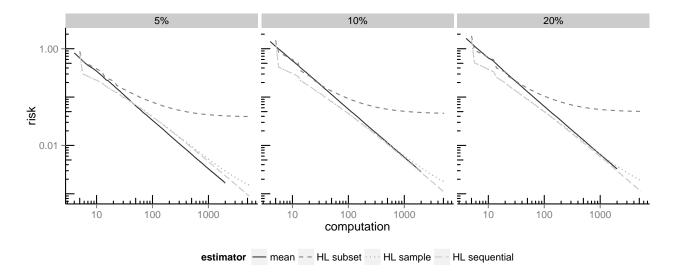


Figure 3: Computation and risk on the log-log scale for the sample mean and variations on the Hodges-Lehmann estimators. The computation is determined by the number of operations to compute the pairwise means and the number of comparisons to compute the median. The three panels correspond to different levels of contamination of 5%, 10% and 20%. At very low costs and very high costs the HL sequential estimator is best but at moder costs, between 100 and 1000, the level of contamination can impact whether the HL sequential estimator or the mean estimator is to be preferred.

In this section we consider the problem of finding the least squares estimator in a standard linear regression

$$Y = X\beta + \epsilon$$

where the columns of X are correlated. Each of the p columns of X represents an attribute of an individual. The solution  $\hat{\beta}=(X^tX)^{-1}X^tY$  is well known and requires the inversion of the Gram matrix  $S=X^tX$ . We explore two iterative methods for matrix inversion. The first is a naive Newton-Raphson (NR) algorithm that inverts the matrix A via the iterative procedure  $A_k^{-1}=2A_{k-1}^{-1}-A_{k-1}^{-1}AA_{k-1}^{-1}$ . It is clear that by letting  $k\to\infty$  we get  $A_k^{-1}\to A^{-1}$  such that  $A^{-1}A=I$  for I the identity matrix.

The second method builds on the power method for eigenvector and eigenvalue approximation. It is well known that the eigenvector associated with the largest eigenvalue of a symmetric matrix A can be computed via the iteration  $v_{k+1}^{(1)} = Av_k^{(1)}/\|Av_k^{(1)}\|_2$  where  $\|\cdot\|_2$  is the squared  $L_2$  norm. To compute the eigenvector associated with the second eigenvalue one

first computes  $v_{\infty}^{(1)}$  and then performs the above iteration replacing A with  $A - v_{\infty}^{(1)} v_{\infty}^{(1)t}$ . A similar expression is available for smaller eigenvalues. We consider several stopping criteria for for this approach. First we consider stopping the computation of the first eigenvector after k steps, then compute the second eigenvector based on  $A - v_k^{(1)} v_k^{(1)t}$  also stopping after k, and so on. A second approach considers stopping the first iteration after k steps, the second after k-1 steps, until the pth after k-p steps.

For the purposes of exposition we consider a matrix  $X = ZD^{1/2}C^{1/2}$  where the entries  $Z_{ij} \stackrel{iid}{\sim} \mathcal{N}(0,1), \ C = (1-\rho)I + 11^t\rho$ , the compound symmetry correlation matrix, and D is a diagonal matrix with entries decreasing uniformly from 4 to 2. As  $\rho \nearrow 1$  the matrix approaches rank deficiency which suggests that for larger values of  $\rho$  algorithms that approximate the inverse via lower rank matrices are likely to perform as well as full rank inversions. In this simulation we consider p=10. The inversion via Newton-Raphson has on the order of  $10^3$  steps, but in practice no more than 20 steps are needed for numeric conversion of the algorithm. The power method approaches have the same algorithmic complexity but converge even faster in practice. Throughout, the true value of  $\beta$  is a uniformly separated sequence from -1 to 1 and we consider the risk of estimating  $\beta$  under quadratic loss. For independent and identically distributed noise  $\epsilon \sim \mathcal{N}(0,1)$  we know that the risk of estimating  $\beta$  is given by  $\sum_i \operatorname{diag}((X^tX)^{-1})_i$  and so we use this exact value to confirm that an inversion method has converged.

We simulate 10,000 datasets in order to estimate the risk for  $\hat{\beta}$  across three values of  $\rho$  between 0.01 and 0.88. In Figure 4 we see the outcomes of the experiment for both types of inversion procedures. For the power method algorithm the computation cost is determined by the total number of iterations of a single run. For example, the linear method costs  $\binom{k+p}{2} - \binom{k}{2}$  iterations, while the approach that stops every iteration after k steps costs kp. Each iteration of NR is assigned a cost of 20 since each one requires two matrix multiplications which involve 20 vector multiplications and each iteration of the power method is a vector multiplication.

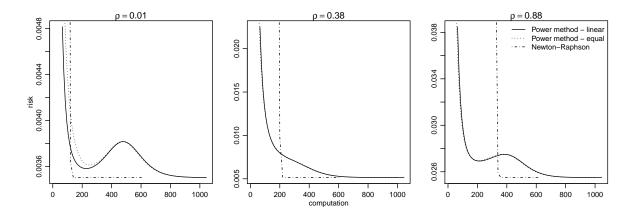


Figure 4: Three plots of simulation results comparing computational cost (as measured by the number of iterations of an algorithm) versus the risk under quadratic loss of estimating the coefficients in a linear regression. Each plot represents a different level of dependence among the columns of the design matrix X.

First it is evident that the risk is reduced non-linearly with increases in computation costs for both methods. The NR algorithm converges to the risk of the fully inverted matrix faster than the two power-method approaches. However it does so at the expense of poor performance before full convergence. In particular, both NR and power-method approaches are initialized naively. While NR has an initial risk (not shown on the plots due to scale) hundreds of times greater than the lowest risk, both power methods are within 30% of the lowest risk after only a few iterations. Throughout the plots we can see that NR is very dependent on the value of  $\rho$  as that determines how well S is approximated by a low rank matrix. The two power-methods appear agnostic to the value of  $\rho$  with the exception of how smoothly they approach the lowest risk. This can be explained by the interdependence between iterations of the power method – that is, a slight improvement in the estimation of the first eigenvector (prior to the convergence of the power method iterations) does not guarantee an improvement in the estimation of the second eigenvector.

#### 7 Conclusions

This article proposed an interpretable framework for the tradeoff between computational cost and statistical risk. Our approach introduced exact computational cost into the analysis of statistical methods. This is first illustrated via the classical example of estimating the mean and variance of a sample of normal random variables. In this setting, we suggest that the use of a single data point for the update of a sufficient statistic should incur a cost of one. This allows us to compute exact and asymptotic risks associated with mean and variance estimation under a computational constraint. We extended this framework to general exponential families in Section 4. We further illustrated our framework in the context of robust estimators (Section 5) and iterative procedures (Section 6).

We note, as we did in Remark 3.2, that we have made simplifying assumptions about the computational costs and runtimes of various procedures. These assumptions allow for the subsequent analysis and we believe are still helpful in guiding the choice of estimators. Sometimes a more detailed and fine-grainded analysis may be desired that does not employ these abstractions. In this case we believe that the practitioner could use benchmarking tools to precisely measure the runtimes of various aspects of their procedures which, together with algorithmic analysis, can be used to employ our framework in choosing the best procedure for the problem at hand.

Beyond the applications presented in this article our approach can be employed whenever computational constraints are present. In the context of experimental design, this framework can inform the number of observations or the number of subjects needed for a study. For high throughput data it can assist in deciding on a sampling mechanism when all data cannot be read into memory. The iterative procedures section suggests the development of analogues to standard methodology (such as linear regression and spectral clustering) that do not necessitate numerical convergence of intermediary steps but that still preserve desirable

statistical properties.

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