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► **To cite this version:**

| Jean-Michel Levy. Is unbiased estimators always justified ?. 2006. hal-00022886v1

HAL Id: hal-00022886

<https://hal.science/hal-00022886v1>

Preprint submitted on 14 Apr 2006 (v1), last revised 5 May 2006 (v2)

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Is unbiased estimators always justified ?

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14th April 2006

Abstract

It is argued that, contrary to common wisdom, unbiasedness is not always a well grounded requirement. It is shown that in many cases, for a given unbiased estimator there is a simply derived biased estimator which yields results closer to the true value.

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1 Introduction and reminder

For the purpose of devising the most efficient way of exploiting them, the results of physical experiments are generally regarded as realisations of random variables; statistical theory is then invoked to indicate efficient ways of using these sets of data for obtaining the values of physical parameters which are functionally tied to the parameters of the probability distributions. In this framework, one calls **estimators** certain random variables built on samples of potential observations which are used to evaluate part or all of the parameters of the underlying ('parent') probability distribution. The sample average is amongst the simplest examples: if the expectation value m of the parent distribution is unknown, the arithmetic mean $\bar{X} = \frac{1}{n} \sum_i X_i$ is the natural and, in many cases, the 'best' estimator that can be found to evaluate m . The word 'best' has been quoted in the preceding sentence for reasons that will soon become 'clearer'.¹

In many cases, the sample is (rightly) assumed to be made of independent observations and -as we shall assume in the sequel- the underlying distribution is supposed to have moments up to second order: there exists an expectation value $E[X] = m$ and a variance $V[X] = E[(X - m)^2] = \mu_2$.² To define our notation, we call A_n the estimator built on a sample of size n and a the parameter to be estimated, but we shall freely drop the subscript when it is irrelevant. We also assume that, as for X , the first two moments of A exist.

1.1 Estimator properties

Since the **estimation**, i.e. the value taken by the estimator after sampling, will be later used in place of the true value a , the one desirable property that A should possess can vaguely be expressed by demanding it to take values as close as possible to a . How closeness is to be measured is the main issue in what follows.

Because it is easier to think in terms of fixed values rather than to keep in mind the full complexity of a probability distribution, one of the first ideas that comes to mind to satisfy this closeness requirement is to look for an estimator the expectation value of which is equal to the unknown parameter: $E[A_n] = a$. Such an estimator is said to be **unbiased**. When the bias (i.e. the difference $b_n = E[A_n] - a$) is not zero, it often happens that it

¹and the word 'clearer' has been quoted for reasons which will pretty soon become obvious (no quotes)

²We use μ_2 rather than the more traditional σ^2 here because we shall be led to use higher moments and a uniform notation is desirable. The centered moment of order k will be called μ_k .

tends to zero when the sample size grows without limit, in which case A_n is said to be **asymptotically unbiased**

At this point, it is important to stress that the only biases considered in the sequel are statistical biases, due to mathematical properties of the estimators. The measurements which are the source of the data can be affected by **systematic** biases for instrumental reasons, a simple example of which being that of a counter which misses part of the 'hits', thereby furnishing a systematically low count. **We assume that this kind of bias is being taken care of by appropriate means and we only address the question of the statistical biases in this article.**

Therefore, over and above unbiasedness, the first quality which is demanded for an estimator is **consistency**: a **consistent estimator** must somehow approach the value to be estimated when n goes to infinity. The precise meaning of the word 'approach' in the previous sentence can vary according to the kind of stochastic convergence which is adopted, but it is usually understood to refer to **convergence in probability**, that is: for **any** given $\epsilon > 0$, the probability that A_n deviates from a by more than ϵ has zero limit when $n \rightarrow \infty$. More formally:

$$\forall \eta > 0 \quad \exists N : \forall n > N \quad P(|A_n - a| > \epsilon) < \eta$$

If $E[A_n]$ has a limit when $n \rightarrow \infty$, one does not see how that limit could differ from a if the previous requirement is fulfilled, but the author knows of no proof of this without additional assumptions.

The rationale for demanding consistency is fairly clear: it is 'obvious' (but can be false !) that averaging a large number of measures of the same quantity will yield a better estimate of that quantity; on the other hand, accumulating data would be of no use if the estimation were not getting closer to the searched for value when the amount of data grows.

It is often written (see e.g.[1]) that asymptotic properties such as consistency have nothing to say for finite sample sizes, contrary to unbiasedness which is a property defined for finite (read: 'realistic') sets of observations. We think statements like this, supposedly based on good old common sense, are very deceiving; indeed, the observed average never equals its expectation value which is also, in a sense, an asymptotic property. All that can be said is that the average of an unlimited number of realisations of A converges to a in some way. (The so-called **law of large numbers**, more on this below) But what is the relevance of all that for a single shot estimation built from a finite sample, especially if A doesn't have a small dispersion ? ³

³Moreover, the standard definition of 'unbiasedness' is quite arbitrary. There is nothing sacred about expectation value and one could as well demand that the median $\mathcal{M}[A_n]$ of the distribution of A_n (defined by $P(A_n \leq \mathcal{M}[A_n]) = P(A_n \geq \mathcal{M}[A_n]) = 1/2$) be equal

Concentration is therefore another important quality and one also demands the estimator to have a 'small' root mean squared that is, $\sqrt{V[A_n]}$ should not be larger than the error one is ready to tolerate on a .

Building estimators with variances going to zero in the infinite sample limit is often possible in simple problems. Ideally, an estimator which is both asymptotically unbiased and of zero asymptotic variance is all that is required, would data be available in arbitrary large amounts: one easily shows that such an estimator is consistent by using Huygen's theorem:

$$E[(A_n - a)^2] = V[A_n] + (E[A_n] - a)^2$$

and Chebyshev's inequality:

$$P(|A_n - a| > \epsilon) < \frac{1}{\epsilon^2} E[(A_n - a)^2]$$

By the same token, one sees that if consistency is understood as convergence in **quadratic mean**, it is completely equivalent to the conjunction of the two asymptotic requirements just stated.

All the insistence on expectation values and sample means comes from the above mentioned law of large numbers, of which there exist weak and strong varieties. For what concerns us, they both say that the arithmetic mean of n equally distributed independent random variables converges in probability (weak law of l.n.) or almost surely (strong law of l.n.) towards their common expectation value when $n \rightarrow \infty$, as soon as this expectation value exists (analytically speaking); this explains why unbiasedness is expressed in terms of expectation values (but see footnote 3) and in simple cases, estimators are indeed averages of this kind for which the law applies. However, although people can gather only finite samples, they tend to believe that their estimators will be 'better' if they are already unbiased for finite sample sizes; they often make big calculational efforts to reach this aim - and spoil their estimators. This is the belief and the practice that we challenge in the following.

2 Why is unbiasedness not necessarily a good idea.

2.1 Smaller variance or smaller bias ?

There is a kind of trade-off between the two requirements of low bias and low variance in certain cases. Let us assume that A_n is multiplicatively biased, by this we mean that $E[A_n] = fa$ where f is some positive number to a . After all, the median of the distribution of the sample median is equal to the median of the parent distribution, call it μ , and the sample median is a consistent estimator of μ for distributions which do not even possess an expectation value (e.g. the lorentzian distribution)

$\neq 1$ which may be a function of n .

If f is known, many practitioners of statistics will rather use $A'_n = \frac{A_n}{f}$. However, the variance of A'_n is $V[A'_n] = \frac{V[A_n]}{f^2}$ and if $f < 1$ one gets unbiasedness at the price of a larger dispersion **and there is no reason to believe that A' is better than A only because its expectation value equals a** . Thinking so is somehow forgetting that a random variable is not its expectation value and unconsciously referring to the law of large numbers, which has, however, nothing to say about the relevance of an asymptotic property for a finite sample.

2.2 What is closer ?

Proximity will be dealt with in terms of distance, or difference. Definitions can vary and if the expected difference between A' and a is indeed zero by construction, the real life difference between the values taken by A' and a is never zero. Therefore it is more realistic to measure their distance by the mean absolute difference or the (root) mean square difference which is easier to handle, that is $D^2(A', a) \equiv E[(A' - a)^2]$ which is simply $V[A']$ for unbiased A' .

As for A , Huygens' theorem says that: $D^2(A, a) = V[A] + (E[A] - a)^2$ The variance is the minimum of the mean square distance about a fixed point, and this minimum is reached for the fixed point taken at the expectation value. Therefore, if A were additively biased, subtracting off the bias would be the right thing to do. But this is not what we have in mind here.

For A' , the squared distance to a is $V[A'] = \frac{V[A]}{f^2}$

For A , it is $V[A] + a^2(1 - f)^2$

The latter can be smaller than the former for $f < 1$ ⁴ and we shall base on this remark a general prescription for improving estimators, but before so doing, let us examine a specific and well known example.

2.3 A simple example

When it is required to estimate the variance of a distribution, the mean of which is unknown, an 'obvious' estimator is the sample variance:

$S^2 = \frac{1}{n} \sum_i (X_i - \bar{X})^2$. However, this S^2 is biased: $E[S^2] = \frac{n-1}{n} \mu_2$ which is precisely the kind of situation that we are considering here. More often than not, people replace S^2 by $S'^2 = \frac{1}{n-1} \sum_i (X_i - \bar{X})^2 = \frac{n}{n-1} S^2$ which has obviously a larger dispersion.

To study the case further, let's make things simple and assume that the parent (sample) distribution is gaussian. (The case of an arbitrary distribution will be treated later)

⁴On the contrary $f > 1$ would entail a larger dispersion of A around a and is therefore uninteresting.

S^2 is then the estimator of μ_2 given by the maximum likelihood method when m is unknown, but again, most people shift to S'^2 because of the bias. However, it is particularly simple to show that one increases the dispersion of the estimator about μ_2 by using this recipe ⁵.

Indeed, it is well known that $Q = \frac{nS^2}{\mu_2}$ is χ^2 -distributed with $n - 1$ degrees of freedom. Therefore $E[Q] = n - 1$, $V[Q] = 2(n - 1)$ and one has $E[S^2] = \frac{n-1}{n}\mu_2$ as it has to be, $V[S^2] = \frac{2(n-1)}{n^2}\mu_2^2$ and $V[S'^2] = \frac{2}{n-1}\mu_2^2$

But this entails that

$$D^2(S^2, \mu_2) = V[S^2] + \mu_2^2\left(\frac{1}{n}\right)^2 = \frac{2n-1}{n^2}\mu_2^2 < V[S'^2]$$

S^2 is therefore **less dispersed about** μ_2 than S'^2 and it makes little sense to prefer the latter on the grounds that it is unbiased. We can only disagree with, e.g. [3] who compare the bias with the loss in precision calculated as the difference between the standard deviations of the two estimates and settle the matter by claiming that 'for large n this loss is very much smaller than the bias'. These are things that cannot be compared. Of course, our mean square distance criterion makes use of expectation values just as the no bias criterion, *but a small D is much more meaningful than a zero expectation value; since all contributions are positive, they all add up in the calculation of D^2 and the true distance squared, in any given experiment, cannot be much larger than D^2 with any sizeable probability, whereas demanding no bias guarantees nothing of the kind since it can be achieved by compensation of large opposite sign contributions.* ⁶

One can derive limitations on the probability of an absolute difference from bounds on the variance or on the expected **absolute** difference as exemplified by Chebyshev's and Kolmogorov's inequalities. But nobody will ever succeed in deriving such a bound from a bound on the bias..to put it otherwise, the absolute value of the integral of a function has much less to say about the size of that function than the integral of its absolute value.

2.4 The weight of habits

Clearly, using S^2 will lead to average estimations below the true value of μ_2 in the long run and the histogram built with many realisations of the Monte Carlo will not be 'centered' on the input value; many people would not like

⁵Quite apart from these considerations, the case for S^2 is sometimes pleaded on the grounds that it is the maximum likelihood estimator among all those samples which have averages equal to the value of \bar{X} which has been found. See [2]

⁶Think of an unbiased estimator with a U-shaped probability distribution function ! This, by the way, is what vindicates the demand for consistency.

using S^2 precisely for that reason. We think the right answer is a flat: 'So, what ?' The real question is: what are those estimates supposed to be used for ? If it is not to show colleagues how well you do in reconstructing the input parameters of your Monte-Carlo, then such things as those histograms should not be considered as the primary criterion in assessing the quality of your estimators. People are taught and used to look at those features, but a minute of thought suffices to convince oneself that a centered histogram proves very little. Control histograms can be plotted with unbiased estimators to show that 'everything is understood', but that doesn't validate the estimators for whatever subsequent use is made of the estimates.

On the contrary, every student knows that, except for linear mappings, the expectation value of the transform is not the transform of the expectation value. Therefore, there is no real reason to insist on rigorously unbiased estimations. The perfectly legitimate requirement of being as close as possible to the true value is often contradictory with the 'no-bias' criterion.

To give yet another example: nobody would say that the mean distance to the origin in, e.g., a one dimensional, symmetrical random walk is zero on the grounds that the expectation value of the random walk is zero for even n_{step} . The root mean square is the universally accepted measure of distance, hence the $\sqrt{n_{step}}$ rule.

3 If unbiased doesn't help, what about..overbias ?

3.1 Optimal bias

Having thus set foot in the marshes of heresy, going forward is the only logical attitude. If S^2 , above, is better than S'^2 , what about $n/(n+k)S^2$?

Finding the optimum value of k can be made by direct comparison: let S''^2 stand for the latter estimator Then $(V[S'^2] - D^2[S''^2, \mu_2])/\mu_2^2 = \frac{2}{n-1}(1 - (\frac{n-1}{n+k})^2) - (\frac{k+1}{n+k})^2 = \frac{k+1}{(n-1)(n+k)^2}(3n + 3k - nk - 1)$

The largest difference obtains for $k = 1$ and is equal to $\frac{4}{n^2-1}\mu_2^2$ The most 'concentrated' estimator about μ_2 is therefore $S''^2 = \frac{1}{n+1} \sum_i (X_i - \bar{X})^2$ This result is but a particular case of a more general formula that will be derived below.

3.2 A word about error compensation

Since the most 'concentrated' estimator of μ_2 is $S''^2 = \frac{1}{n+1} \sum_i (X_i - \bar{X})^2$ and since this is probably not unknown, one might ask why people keep on using the unbiased S'^2 instead. Besides the already alluded to histograms, the unconscious idea underlying the use of unbiased estimates is probably that fluctuations above and below the 'true value' (which is the expectation value of S'^2 in this case) should more or less compensate. We have

already remarked that such a motivation is poorly grounded for a one-time estimation. But for the sake of the argument, let us take the idea seriously. The best estimator in that case should be such that its probability to be above the 'true value' is equal to its probability to be below this value. In other words, for our example, μ_2 should be the **median** of the distribution of the estimator rather than its mean. Let's therefore define an 'ideal' S_{id}^2 proportionnal to S'^2 such that μ_2 be the median of its distribution. Let $S_{id}^2 = \alpha S'^2$. Then $\frac{(n-1)}{\alpha \mu_2} S_{id}^2$ is χ^2 distributed with $n - 1$ d.d.f. and the condition we impose calls for finding the median \mathcal{M}_{n-1} of the χ^2 distribution. Numerical evaluation up to $n = 400$ shows that the median of χ_n^2 is always between n and $n - 1$, slowly decreasing and seemingly converging towards $n - 2/3$ but this value is, of course, only a guess. This means that $\alpha = \frac{n-1}{\mathcal{M}_{n-1}} > 1$ and therefore that S_{id}^2 is not below but above S'^2 contrary to the conclusion to which we were led by our distance argument. One has $S_{id}^2 = \frac{1}{n-r} \sum_i (X_i - \bar{X})^2$ with $r \approx 5/3$ and the (mean squared) distance between S_{id}^2 and μ_2 is $V[S_{id}^2] + (\frac{r-1}{n-r})^2 \mu_2$, larger than everything found so far.

Facing this distressing result, one might think of a last way out for the case at hand: in the same spirit as our tentative use of the median and in line with the philosophy of the maximum likelihood method, one could assume that the best estimate of μ_2 is that which renders the value found for S'^2 most likely. Contrary to the median case, it is quite easy to find by derivation that the most likely value (the so-called '**mode**') of a χ_n^2 distribution is $n - 2$. Therefore the maximum likelihood estimator of μ_2 **in this sense** should be taken as $\frac{n-1}{n-3} S'^2 = \frac{1}{n-3} \sum_i (X_i - \bar{X})^2$, still farther away from S^2 than the preceding estimate (recall that S^2 **is** the maximum likelihood estimate for a gaussian sample with unknown mean). The maximum likelihood method seems therefore to suffer of some kind of schizophrenia: the maximum likelihood estimator of μ_2 based on the full sample distribution, that is S^2 , is not the same as the maximum likelihood estimator of the **same** parameter based on the distribution of this **same** S^2 , which is $\frac{n}{n-3} S^2$..

4 A general prescription

4.1 Improving an unbiased estimator

The lesson of the latter section is that 'compensation' arguments lead only to contradiction. Even the time honored maximum likelihood method is shown to be self-inconsistent. Aware of this fact, some people use M.L. only as a starting point to find some estimator which they further 'improve'. But as already remarked, the supposed improvement can spoil the result and this is particularly clear on the example that we have used.

On the other hand, the minimum squared distance criterion is certainly better grounded than the no-bias prescription for reasons which have already been explained. One then might ask for a general rule based on it. Using the notations of paragraph 2.2, the squared distance of A to a can be written:

$$D^2(A, a) = V[A] + (E[A] - a)^2 = f^2V[A'] + a^2(f - 1)^2$$

Therefore, having found an unbiased estimator A' one can try to derive a smaller distance estimator by minimizing the above expression w.r.t. f . Zeroing the derivative yields the condition:

$$f = f_m \equiv \frac{a^2}{E[A'^2]}$$

where use has been made of $V[A'] = E[A'^2] - a^2$. Since $a^2 = E[A']^2 < E[A'^2]$, $f_m < 1$ as expected. Starting from any unbiased A' , it is always possible to build, in principle, an improved estimator:

$$A_{better} = \frac{a^2}{E[A'^2]}A'$$

which will be closer to the unknown parameter than A' . It is, of course, biased, but its squared distance to a is easily seen to be reduced by a factor of f_m

Note that, at least for 'mean square' consistency, $f_m \rightarrow 1$ when $n \rightarrow \infty$ because convergence in the mean square entails convergence of the first two moments of the distribution towards those of a constant; in particular, $E[A'_n{}^2] \rightarrow E[a^2] = a^2$ so that as soon as they are built from consistent estimators, our biased estimators are themselves consistent.

The expression found for A_{better} seems to depend on the value to be estimated. However, although there exist indeed cases in which it is of no use, we'll see presently that there are some important simple problems where it is perfectly usable.

Moreover, even if the exact value is not known, any non trivial upper bound on f_m (that is, smaller than 1) will yield some improvement if used in place of f_m to bias A' .

It is important to observe here that the bias so introduced always tends to zero when $n \rightarrow \infty$ as soon as the (unbiased) estimator variance goes to zero. Indeed, $f_m = \frac{a^2}{V[A'] + a^2} \rightarrow 1$ in this case.

4.2 Examples

- Estimation of the variance of a gaussian distribution with unknown expectation value.

This is the already treated example. Here $a = \mu_2$ and $E[A'^2] = V[S'^2] + \mu_2^2 = \frac{2}{n-1}\mu_2^2 + \mu_2^2$ therefore $f = \frac{n-1}{n+1}$ and $S_{better}^2 = \frac{1}{n+1} \sum_i (X_i - \bar{X})^2$ as already found.

- Estimation of the variance of a gaussian distribution with known expectation value.

The unbiased estimator is here $S_0^2 = \frac{1}{n} \sum_i (X_i - m)^2$

with $V[nS^2/\mu_2] = 2n$ hence $V[S_0^2] = \frac{2\mu_2^2}{n}$

Therefore $f = \frac{n}{n+2}$ and $S_{better}^2 = \frac{1}{n+2} \sum_i (X_i - m)^2$

- Estimation of the variance of an arbitrary distribution with known expectation value.

With S_0 as here above for the unbiased estimator one finds:

$$E[(S_0^2)^2] = \frac{1}{n^2} E\left[\sum_i (X_i - m)^4 + 2 \sum_{i < j} (X_i - m)^2 (X_j - m)^2\right] = \frac{1}{n} \mu_4 + \frac{n-1}{n} \mu_2^2$$

The improved estimator is therefore: $S_{better}^2 = \frac{n}{\gamma+n-1} S_0^2$ with γ the ratio $\frac{\mu_4}{\mu_2^2}$ (γ equals 3 for a gaussian distribution, which checks our preceding result).

- Estimation of the variance of an arbitrary distribution with unknown expectation value.

This calls for the more tedious calculation of the second moment of S'^2 defined above. One finds $E[(S'^2)^2] = \frac{\mu_4}{n} + \frac{n^2-2n+3}{n(n-1)} \mu_2^2$ and the improved estimator can be written:

$$S_{better}^2 = \frac{n}{\gamma + n - 1 + \frac{2}{n-1}} S'^2$$

Note that by Schwartz's inequality, $\gamma > 1$ in accordance with our calculations for the last two items. The second result yields a marginal improvement even in the absence of a better knowledge of γ than this trivial bound.

- Estimation of the parameter of an exponential distribution.

The density is $\frac{1}{\tau} e^{-\frac{t}{\tau}}$ for $t > 0$ and the unbiased estimator of τ is $\hat{\tau} = \frac{1}{n} \sum_i T_i$ with variance $\frac{\tau}{n}$ One finds $\hat{\tau}_{better} = \frac{1}{n+1} \sum_i T_i$

- If, in the preceding exemple, one prefers to estimate the rate $\lambda = \tau^{-1}$, the M.L. estimator is $\hat{\lambda} = \frac{n}{\sum_i T_i}$ The moments of $\hat{\lambda}$ are easily computed by observing that $\frac{n}{\hat{\lambda}}$ is distributed according to a $\gamma(n, \lambda)$ law and by using the normalisation integral:

$\Gamma(k) = \int_0^\infty x^k \lambda^{k-1} e^{-\lambda x} dx$. $\hat{\lambda}$ is biased but $\frac{n-1}{n} \hat{\lambda}$ is not and one finds that the improved estimator is $\hat{\lambda}_{better} = \frac{n-2}{n} \hat{\lambda}$

- For an unbiased estimator which reaches the minimum variance bound (Cramer-Rao inequality), the factor f_m reads $\frac{a^2}{a^2+1/I_n(a)} = \frac{a^2 I_n}{1+a^2 I_n}$ where I_n is the amount of information on a brought by the n -sample, viz: $I_n(a) = E[(\frac{\partial \text{Log} \mathcal{L}}{\partial a})^2]$ with \mathcal{L} the likelihood of the sample. The lifetime estimator above is a case of that kind.
- For a last example, let us consider the maximum likelihood estimator of the parameter θ of a uniform distribution on $[0, \theta]$. This is $\hat{\theta} = \text{sup}_i X_i$ where the $\{X_i\}$ stands for the sample. This estimator is easily shown to be biased: $E[\hat{\theta}] = \frac{n}{n+1}\theta$. The unbiased estimator is therefore $\frac{n+1}{n}\text{sup}_i X_i$ from which one easily finds the improved $\theta_{\text{better}} = \frac{n+2}{n+1}\text{sup}_i X_i$

5 Summary and conclusion

It has been argued that the requirement of unbiasedness at the price of a larger mean square distance to the estimated parameter is not well grounded. Mean absolute differences or mean squared differences are clearly more meaningful than the average of signed differences which can hide large fluctuation through compensation. It has been observed that the demand of a 'centered' histogram is a matter of habit, but has no meaning as to the optimality of the estimates for other purposes than checking calculations. Requiring histograms to be 'centered' in reference to the median would not be less legitimate.

However, with the help of a definite example, it has been shown that attempts to use some kind of fantasmatic 'error compensation' through the use of mean, median or mode leads to contradictions and to the use of estimators with ever wider distributions.

On the other hand, minimizing the mean square distance gives a general prescription to improve on an unbiased estimator by biasing it to a slightly lower expectation value. Even if the formula for the bias factor thus obtained is not always applicable because of the unknown quantities that it involves, it has been shown that it yields perfectly definite and usable results in some important cases. Any non trivial upper bound on this bias factor yields some improvement.

In conclusion, unbiased estimators are certainly usefull for constructing control histograms, but should not be automatically taken at face value when the problem is that of using the estimates for further calculations.

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