Calibrating the scan statistic with size-dependent critical values: heuristics, methodology and computation

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Abstract

It is known that the scan statistic with variable window size favors the detection of signals with small spatial extent and there is a corresponding loss of power for signals with large spatial extent. Recent results have shown that this loss is not inevitable: Using critical values that depend on the size of the window allows optimal detection for all signal sizes simultaneously, so there is no substantial price to pay for not knowing the correct window size and for scanning with a variable window size. This paper gives a review of the heuristics and methodology for such size-dependent critical values, their applications to various settings including the multivariate case, and recent results about fast algorithms for computing scan statistics.

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1 Introduction

The scan statistic is the standard tool for detecting a signal that may be present at an unknown location in a sequence of observations or in a random field. There has been a considerable recent growth in the popularity of the scan statistic due to the emergence of related problems that involve the detection of anomalies in e.g. sensor arrays and digital images, see Arias-Castro et al. (2011) for further examples. It turns out that several key methodological issues that arise in these diverse settings are already present in a simple univariate sequence model and that the solutions derived there can often be readily transferred to these more involved settings. It is therefore helpful to focus on the simple univariate model where we observe

\[
Y_i = \mu 1(j \leq i \leq k) + Z_i, \quad i = 1, \ldots, n
\]

where the \(Z_i\) are i.i.d. \(N(0,1)\) and both the mean \(\mu\) and the support \([j, k]\) are unknown. The task is to decide whether an elevated mean is present, i.e. to test \(\mu = 0\) vs. \(\mu > 0\) when the support \([j, k]\) is unknown.

The scan statistic arises in this setting using a standard statistical approach as follows: The log-likelihood ratio statistic for testing \(\mu = 0\) when the support \([j, k]\) is known is computed to be \(\frac{1}{2}(\sum_{i=j}^{k} Y_i)^2/(k - j + 1)\). Since \([j, k]\) is unknown, maximizing over \(j\) and \(k\) yields the generalized likelihood ratio test statistic

\[
M_n = \max_{1 \leq j \leq k \leq n} \frac{\sum_{i=j}^{k} Y_i}{\sqrt{k - j + 1}},
\]

which is the scan statistic. It should be noted that the scan statistic was originally defined for a fixed window width \(k - j\), see Glaz et al. (2001), but as pointed out in Cressie (1977), Loader (1991), Nagarwalla (1996) and Kulldorff (1997), the window width is typically not known and therefore also needs to be maximized over \(k\). Note that treating the window width as unknown would seemingly greatly increase the multiple testing penalty of the problem as in addition to scanning over the unknown location \(j\) one also has to scan over the unknown width \(k - j\). It is a rather recent and perhaps surprising finding that scanning over an unknown window width can be done in a way that does not result in a substantial loss of detection power when compared to the case where the correct window width is known a priori. In other words, while there is a price to pay for scanning over locations, there is no further substantial penalty for scanning over the unknown window width, provided that the scan is calibrated in an appropriate way. This review paper describes different methods for such a calibration and gives some heuristic understanding of the theoretical results in the literature that motivate such an approach.

Scan statistics appear in different stochastic settings. In fact, one of the first problems that motivated the use of the scan statistic was the detection of time intervals with an unusually large number of events, see Glaz et al. (2001). While the technical work required in the latter setting is different from that in the Gaussian model \([1]\), it turns out that the heuristics and general ideas described below apply just as well, and theoretical results are remarkably similar in these different settings. Section \([2]\) describes how these heuristics apply to some of these situations. Computing the scan statistic becomes a critical issue in the multivariate setting, and the past decade has seen important work in that regard which is summarized in Section \([6]\). One key result is that computing certain multivariate scan statistics is not subject to the curse of dimensionality. That is, there are algorithms that compute a sufficiently precise approximation to the scan statistic with a time complexity that is almost linear in the number of observations. This unexpected result has the potential to shift the direction of future research.

\[1\] In recognition of this historical precedent Sharpnack and Arias-Castro (2016) call \(M_n\) the multiscale scan, but this paper will simply refer to \(M_n\) as the scan.
statistical work on the scan statistic, which in the last 50 years was focused on deriving its exact or approximate null distribution: Fast algorithms make it possible to efficiently simulate this null distribution, thus moving the focus of research to constructing such algorithms for the particular setting at hand, and to other methodological problems such as how to combine the evidence from various scan windows in a way different from (2). In fact, it is another interesting finding emerging in the last decade that good solutions to the computational and statistical problems often rest on the same key ideas, as will be seen below.

2 Heuristics for calibrating the maximum

While the scan statistic (2) enjoys a simple form and is motivated as generalized likelihood ratio test, it was observed that it is very sensitive for very small window sizes at the expense of moderate and larger window sizes, see Naus and Wallenstein (2004), Neill (2009) and Chan (2009). Naus and Wallenstein (2004) propose to remedy this situation by first finding the cluster size (window width) $w$ that results in the smallest p-value $p_w$ (computed for this single $w$), and then taking as overall p-value the probability that any cluster of smaller or equal size will have a p-value smaller than $p_w$ under the null hypothesis. A detailed investigation of the performance of this method is still outstanding. This exposition will focus on different ways to address the calibration problem that have become increasingly popular in the last decade.

In order to understand the problem at hand it is helpful to rewrite the scan (2) as

$$M_n = \max_{1 \leq w \leq n} L_w,$$

where $L_w = \max_{1 \leq j \leq n+1-w} \sum_{i=j}^{i+w-1} Y_i / \sqrt{w}$ is the maximum over all windows with width $w$. The standard use of the scan rejects $H_0 : \mu = 0$ if $M_n$ exceeds its critical value $q_n(\alpha)$, which is defined under $H_0$ via

$$\mathbb{P}_0(M_n > q_n(\alpha)) = \alpha$$

for a given significance level $\alpha \in (0, 1)$. Note that this implies that all $L_w$ are referred to the same critical value $q_n(\alpha)$. But it is readily seen that one can as well use critical values that depend on the window width $w$: Any vector $\{q_{n,w}(\alpha), w = 1, \ldots, n\}$ that satisfies

$$\mathbb{P}_0(L_w > q_{n,w}(\alpha) \text{ for some } w \in \{1, \ldots, n\}) \leq \alpha$$

will result in a test that has level $\alpha$. The motivation for using such size-dependent critical values derives from a desire to counteract the abovementioned observation that $M_n$ is very sensitive to small window sizes at the expense of moderate and larger window sizes. While it is clear from (5) that size-dependent critical values allow to trade off the sensitivity of various window sizes, it would also appear from (5) that such a trade-off is a zero-sum game: Lowering $q_{n,w}(\alpha)$ (and therefore increasing the power of $L_w$) for some $w$ necessarily requires increasing some of the other $q_{n,w}(\alpha)$ in order to keep the significance level $\alpha$, therefore reducing the power of those $L_w$. Surprisingly, it is possible to construct $q_{n,w}(\alpha)$ such that this trade-off is not a zero-sum game but nearly a ‘free lunch’: it is possible to substantially increase the power for moderate and large window sizes at the cost of a very small (and asymptotically disappearing) power loss for small window sizes. Before describing relevant methodology we give a heuristic explanation of the underlying idea, which exploits the concentration of Gaussian maxima:
Consider the smallest window size $w = 1$. Then $L_w$ is the maximum of $n$ i.i.d. standard normals, and this maximum is known to be very close to $\sqrt{2 \log n}$, see e.g. Leadbetter et al. (1983). An analogous conclusion holds for larger window sizes $w > 1$: since there are about $\frac{n}{w}$ abutting and hence disjoint windows, there are about $\frac{n}{w}$ independent standard normals in $L_w$. Their maximum is close to $\sqrt{2 \log \frac{n}{w}}$. This remains true for the maximum over all (overlapping) intervals of length $w$ because the corresponding test statistics are strongly correlated with the $\frac{n}{w}$ independent ones. Therefore the distribution of (3) is dominated by small windows with $w \approx 1$ and concentrates around $\sqrt{2 \log n}$. This explains the observation by Naus and Wallenstein (2004) that the scan is sensitive for very small windows at the expense of moderate and larger window sizes: The null distribution of $L_w$ is close to $\sqrt{2 \log \frac{n}{w}}$, but the null distribution of $M_n$ will concentrate around $\sqrt{2 \log n}$, thus resulting in a power loss for larger windows.

But the above heuristic also suggests a way to remedy this problem: It suggests that one can increase $L_w$ by as much as $\sqrt{2 \log n} - \sqrt{2 \log \frac{n}{w}}$ without increasing the maximum $M_n \approx \sqrt{2 \log n}$, provided that $L_w$ is concentrated closely around $\sqrt{2 \log \frac{n}{w}}$. The consequence of this would be an increase in power for larger window sizes $w$; in fact, the resulting critical value for $L_w$ would be $\sqrt{2 \log \frac{n}{w}}$, which is the same critical value we would obtain for $L_w$ if we tested the window size $w$ only. In other words, there would be no multiple testing penalty for considering multiple window sizes $w$ in the thus modified $M_n$.

This heuristic suggests to calibrate the scan via

$$\tilde{M}_n := \max_{1 \leq w \leq n} \left( L_w - \sqrt{2 \log \frac{n}{w}} \right).$$

This results in size-dependent critical values for $L_w$ of the form

$$q_{n,w}(\alpha) = \sqrt{2 \log \frac{n}{w}} + \kappa_n(\alpha)$$

where $\kappa_n(\alpha)$ denotes the $(1 - \alpha)$-quantile of $\tilde{M}_n$. This choice ensures that (5) holds, i.e. the resulting test has level $\alpha$. The penalty term $\sqrt{2 \log \frac{n}{w}}$ appears to have been first introduced by Dümbgen and Spokoiny (2001) in the context of function estimation.

### 2.1 Asymptotic optimality theory and finite sample performance

The heuristic derivation of the solution (7) to the problem (5) of finding size-dependent critical values can be backed up with a theoretical optimality result. This result was established by Dümbgen and Spokoiny (2001) in the different context of testing certain features of a function. In the context of the scan problem (1), this result states that the calibration (7) results in asymptotic power 1 against alternatives

$$\mu = \mu(n, w) \geq (\sqrt{2} + \epsilon_n) \sqrt{\frac{\log \frac{n}{w}}{w}},$$

provided that $\epsilon_n$ is not too small: $\epsilon_n \sqrt{\log \frac{n}{w}} \to \infty$. On the other hand, they show that if $\sqrt{2} + \epsilon_n$ is replaced by $\sqrt{2} - \epsilon_n$, then no test can exist that will detect this alternative with nontrivial asymptotic power in the minimax sense. Thus there is a sharp cutoff below which detection is not possible, while above the cutoff $\tilde{M}_n$ has asymptotic power 1 and is therefore optimal. It can be shown that these thresholds also apply if the window size $w$ is known a priori, in which case no multiple testing across various $w$ is required. Therefore this result formalizes the above heuristic finding that the calibration (7) avoids the multiple testing penalty for considering
multiple window sizes $w$, at least in a large sample setting. This above sharp cutoff applies to small window sizes, i.e. $\frac{n}{w} \rightarrow \infty$. A complementary optimality result for larger window sizes, i.e. $\limsup \frac{n}{w} < \infty$, shows that the above condition (8) is necessary for asymptotic power 1, see Dümbgen and Walther (2008) and Datta and Sen (2018). Note that in that case (5) becomes $\mu \sqrt{n} \rightarrow \infty$, which is the parametric rate for detecting an elevated interval, as one would expect.

In contrast, it was shown in Chan and Walther (2013) that the regular scan statistic $M_n$ in (2) will not attain these optimal thresholds except for the very smallest window sizes.

The theoretical optimality results described above concern the large sample setting. However, simulations show that the finite sample performance of the calibration (6) is often unsatisfactory as it is very sensitive for large windows at the expense of very small windows, i.e. it overcompensates the shortcoming of the scan $M_n$, see Rufibach and Walther (2010), Sharpnack and Arias-Castro (2016) and Walther and Perry (2019). The reason for this overcompensation is a consequence of Gaussian concentration around the maximum: $L_w = \sqrt{2 \log \frac{n}{w} + o_p(1)}$, where the $o_p(1)$ term becomes small as $\frac{n}{w} \rightarrow \infty$. So for larger window sizes the $o_p(1)$ term need not be small, and in fact will not be small. Therefore, the null distribution of $\tilde{M}_n$ will essentially be determined by the large windows, with a resulting loss of power for very small windows that is not adequately captured by the asymptotic optimality theory. See Walther and Perry (2019) for simulations that detail this effect. They also explain why the asymptotic optimality theory described above will necessarily be too imprecise to evaluate the performance of a calibration with an appropriate level of prevision, even in the large sample context. In summary, the asymptotic optimality theory available at the time of this writing provides a condition that is necessary but not sufficient for a good performance.

In lieu of evaluating the performance of a calibration via asymptotic optimality, Walther and Perry (2019) propose a finite sample criterion: the realized exponent measures how close the calibration comes to attaining the asymptotic detection boundary in the finite sample situation at hand. This is especially relevant in a multivariate situation, where asymptotic results for the massive multiple testing problem involved in scanning appear to be a poor indication of the performance in a finite sample situation, see Section 5.

3 Methodology for calibrating the scan statistic

This section describes methodology that results in improved power for larger windows vis-a-vis the scan (3) as motivated by the above heuristics, while largely avoiding the overcompensation (i.e. loss of power at small $w$) of (6).

1. The Sharpnack-Arias-Castro calibration

Walther and Perry (2019) report that a modification of a penalty introduced by Sharpnack and Arias-Castro (2016), namely

$$ SAC_n = \max_{1 \leq w \leq n} \left( L_w - \sqrt{2 \log \frac{en}{w} (1 + \log w^2)} \right) $$



gives the desired improvement to (6): It results in better detection power for larger windows than the scan (3), while sacrificing only a slight amount of power at small windows. As in the case (6), the Sharpnack-Arias-Castro calibration results in size-dependent critical values for $L_w$, which are now of the form

$$ q_{n,w}(\alpha) = \sqrt{2 \log \frac{en}{w} (1 + \log w^2)} + \kappa_n(\alpha) $$

\[5\]
where $\kappa_n(\alpha)$ now denotes the $(1 - \alpha)$-quantile of $SAC_n$. This quantile $\kappa_n(\alpha)$ can be obtained by simulation, resulting in finite sample confidence statements.

The Sharpnack-Arias-Castro calibration is closely related to the Dümbgen-Spokoiny calibration (6), but in the former case the penalty term is larger for larger window sizes, thus assigning more power to small window sizes. In fact, Dümbgen and Spokoiny (2001) give a refinement of their penalty that aims for the same outcome by introducing an iterated logarithm term. However, Walther and Perry (2019) report that this refinement has a performance that is nearly indistinguishable from (6) for sample sizes up to $10^6$.

Note that the Sharpnack-Arias-Castro calibration is tailor-made for the Gaussian setting (1), not only because of the simulation of the quantile $\kappa_n(\alpha)$, but importantly the penalty term in $SAC_n$ will produce a good distribution of power across the window lengths $w$ specifically in the (sub-)Gaussian case, without any guarantee for a reasonable performance for other distributions. If one wishes to use $SAC_n$ for different settings and retain its good performance, then it is necessary to employ a test statistic that has sub-Gaussian tails under the null hypothesis, or to transform the test statistic $\sum_{i=j}^{k} Y_i$ to this effect. Fortunately, this is possible in many important cases. Walther (2021) gives a number of ways to standardize sums in order to obtain sub-Gaussian, or even Gaussian, tail bounds, e.g. by working with the square root of the log likelihood ratio statistic in the case of exponential families, see also Rivara and Walther (2013), Frick et al. (2014), König et al. (2018); by employing self-normalized sums in the case of symmetric distributions; or by working with statistics based on ranks in the case of exchangeable random variables.

Of course, constructing a test statistic that has sub-Gaussian tails under the null is not sufficient for a good performance, the particular test statistic must also result in good detection power. This has to be established in each setting with theory or with simulations.

2. The blocked scan

All of the preceding solutions to the calibration problem (5) use an explicit specification of the critical values $q_{n,w}$. A different approach is given in Walther (2010), who proposes to calibrate the significance levels of the various window sizes rather than the critical values. The idea is that by directly controlling these significance levels one can ensure a desirable trade-off between small and large windows in a quite general way that is not specific to the Gaussian setting; recall that the penalty terms above were derived for the Gaussian setting and different distributional assumptions would require a different penalty.

The idea of the blocked scan is to group intervals of roughly the same length (e.g. having length within a factor of 2) into a block. Then all intervals within a block are assigned the same critical value. This critical value is set so that the significance level for the block is proportional to a harmonic sequence (i.e. a harmonic sequence in the block index when the blocks are indexed by increasing window size). We refer the reader to Walther and Perry (2019) for the details. Simulations and theory in Walther (2010) and Walther and Perry (2019) show that this calibration performs similarly to the Sharpnack-Arias-Castro calibration in the Gaussian case and that it possesses asymptotic optimality properties.

The blocked scan has the advantage that it provides a quite general recipe that is neither wedded to a distributional assumption nor to the univariate setting, and which has also proven useful in related testing problems, see e.g. Rufibach and Walther (2010). On the other hand, the blocked scan requires to obtain the quantiles for each block by simulation, and the number of simulation runs will be larger than for e.g. (6) since one needs to simulate multiple quantiles. This is being facilitated by the development of fast approximations to the scan statistic, in particular in the multivariate setting, that are described in Section 6.
Another key point for an efficient simulation is the fact that the number of blocks is small, of the order \( \log_2 n \), due to the grouping of intervals by length within a factor of 2.

An alternative to simulating the quantiles of each block would be to use a model for their distribution. Results by Siegmund and Venkatraman (1995), Kabluchko (2011) and Sharpnack and Arias-Castro (2016) in the Gaussian model suggest that the distribution of \( \max_{w \in \ell} L_w \) can be approximated by a Gumbel distribution after an appropriate centering and scaling. Then one needs to simulate only one parameter \( \tilde{\alpha} \), which is to be used for all blocks, in order to calibrate the blocked scan to have level \( \alpha \), see Walther (2010) or Walther and Perry (2019). Note that the Gumbel distribution would only be used as a model for the block in order to make it possible to easily balance the contributions of the blocks (i.e. window sizes) to the overall statistic. Even if the approximation via the Gumbel distribution turned out to be poor, the choice of \( \tilde{\alpha} \) will ensure that the test has a valid level \( \alpha \).

3. The Bonferroni scan

Each of the calibrations considered so far, namely (6), (6), SAC, and the blocked scan, involves a maximum, and therefore the null distribution needs to be approximated either analytically or by simulation. The Bonferroni scan avoids this extraneous computation by calibrating the statistic for each window, i.e. \( \sum_{i=j}^{k} Y_i / \sqrt{k-j+1} \), with a weighted Bonferroni adjustment. At first glance it would appear that applying a Bonferroni correction to the \( \sim n^2 \) windows \((j,k)\) in model (1) is ill-advised as it would lead to a hopeless loss of power - even more so in a \( d \)-dimensional setting, where the number of rectangles grows like \( n^{2d} \). However, work in the last 15 years has shown that it is possible to effectively approximate the maximum of these \( \sim n^2 \) statistics \( \sum_{i=j}^{k} Y_i / \sqrt{k-j+1} \) by evaluating them on a judiciously chosen set of only about \( O(n) \) windows. The Bonferroni scan exploits this fact not only for fast computation, but also for inference: Since it suffices to consider a sparse collection of relatively few windows, there is hope that a simple Bonferroni adjustment will lead to critical values that result in good performance. It was shown in Walther and Perry (2019) that this is indeed the case: Using a certain weighted Bonferroni adjustment leads to a performance in terms of detection power that is asymptotically optimal, and almost as good as that of the Sharpnack-Arias-Castro calibration and the blocked scan in a finite sample setting. In fact, the mechanics of the weighted Bonferroni adjustment are very similar to the blocked scan: Windows are grouped into blocks according to their length and the Bonferroni adjustment includes a weight that is proportional to a harmonic sequence. The choice of the approximating set of windows is crucial for a good performance of the Bonferroni scan. This requires to strike a delicate balance in order to guarantee a good detection power: the collection of windows has to be rich enough so it can provide a good approximation for an arbitrary window \((j,k)\), but it also has to be sparse enough so that a Bonferroni adjustment will not unduly diminish the detection power. The main idea is that instead of evaluating all windows \((j,k)\), \( 0 \leq j < k \leq n \), one considers only endpoints on a grid \( \{id_\ell, i = 0, 1, 2, \ldots\} \), where the spacing \( d_\ell \) has to increase with the window length \( \ell \) at a certain rate. See Section 6 and Walther and Perry (2019) for the details.

For all of the above three calibrations, the improved performance compared to (6) is achieved by relenting somewhat on the demand for optimality for the largest windows \( w \approx n \), which is presumably not an important concern in practice. For example, the penalty in SAC will not stay bounded for large windows and hence the optimality result for large windows will not hold any more. But for these large windows the penalty grows only at the very slow rate \( \sqrt{\log \log n} \), which should result in only a small loss of power.
With the exception of the Bonferroni scan, all of the calibrations discussed so far involve terms that need to be approximated analytically or by simulation, such as $g_n(\alpha)$ for the traditional scan (4) or $\kappa_n(\alpha)$ for (7) or (9). There exist large sample approximations to the critical values of several of these calibrations, see Siegmund and Venkatraman (1995), Kabluchko (2011), and Sharpnack and Arias-Castro (2016). However, Sharpnack and Arias-Castro (2016) find that these approximations are often too conservative, and they recommend instead to approximate these critical values with simulations or permutation tests. Such simulations and permutation tests can often be rigorously justified, see e.g. Walther (2010), Rivera and Walther (2013), or Arias-Castro et al. (2018), and are made possible by recent advances that allow for a fast computation of the scan statistic, see Section 6.

4 Related settings

As mentioned in Section 1, scan statistics often arise in settings that are different from the Gaussian sequence model (1). Of particular interest in literature is the setting where one observes an (in)homogeneous Poisson process and the problem is to detect an interval where the intensity is elevated compared to a known baseline, i.e. one is looking for an interval with an unusually large number of events, see Glaz et al. (2001). Conditioning on the total number of observed events allows to eliminate certain nuisance parameters and shows that the problem is equivalent to testing whether $n$ i.i.d. observations arise from a known density $f_0$ (which w.l.o.g. can be taken to be the uniform density on $[0,1]$) versus the alternative that $f_0$ is elevated on an interval $I$:

$$f_{r,I}(x) = \frac{r 1(x \in I) + 1(x \in I^c)}{r F_0(I) + F_0(I^c)} f_0(x),$$

so the problem becomes testing $r = 1$ vs. $r > 1$, see Loader (1991) and Rivera and Walther (2013). The results in the latter paper show that the heuristics, methodology and optimality results in the density/intensity model (10) are quite analogous to the Gaussian sequence model (1). However, in order to apply the calibrations from the previous section and to achieve optimal detection, it is critical to set up the methodology correctly. In particular, it was pointed out in Rivera and Walther (2013) that using the square root of the log likelihood ratio statistic together with the calibrations described in the previous section provides a general recipe for optimal detection. That is, just as the statistic $\sum_{i=j}^k Y_i$ in (2) corresponds to the square root of twice the log likelihood ratio statistic in (1), one needs to work with the square root of twice the log likelihood ratio statistic in (10) rather than statistics such as $Y_{(k)} - Y_{(j)}$ which are often used in model (10) to detect clusters of points. The reason why this is important is that the $\sqrt{2\log\ldots}$ penalty term in calibrations such as (7) or $SAC_n$ derives from the Gaussian tail of the statistic $\sum_{i=j}^k Y_i$. But statistics such as $Y_{(k)} - Y_{(j)}$ do not follow a normal distribution under the null hypothesis, and therefore these calibrations will not give satisfactory results. On the other hand, the log likelihood ratio statistic provides a quite general solution to this problem: Not only is log likelihood ratio known to typically provide the most powerful test statistic, but according to statistical folklore twice the log likelihood ratio follows approximately a $\chi^2_1$ distribution, so that one can hope that the square root of twice the log likelihood ratio will have approximately Gaussian tails and therefore calibrations such as those discussed above should provide optimal detection. It was indeed shown in Rivera and Walther (2013) that the square root of twice the log likelihood ratio statistic in (10) satisfies a finite sample sub-Gaussian tail inequality. Therefore, the methodology and optimality results from the Gaussian sequence model (1) can be carried over to the model (10). This transfer of methodology rests on a second key point: The indices $(j,k)$ for the window in (2) correspond to the indices of order statistics in model (10), i.e. the scanning is with respect to the empirical measure rather
than with respect to the sample space. With that identification the scan statistic becomes a process on \( \{1, \ldots, n\} \) rather than on a particular sample space, and the methodology described in the previous sections can be applied quite generally by replacing \( \sum_{k=j}^{k+1} Y_i \sqrt{2 \log \log n} \) with \( \sqrt{2 \log LR(j, k)} \), where \( \log LR(j, k) \) is the log likelihood ratio statistic on the interval \( (Y_j, Y_{(k)}) \).

The square root of the log likelihood ratio statistic has been successfully applied in other contexts, e.g., in Bernoulli model with a random design in Walther (2010), or to data from an exponential family observed at a fixed design in Frick et al. (2014) and in König et al. (2018). In the case of exponential families the crucial sub-Gaussian tail bound for the square root of the log likelihood ratio can be derived by inverting the Cramér-Chernoff bound, see Rivera and Walther (2013) and Walther (2021); or by normal approximation, see Frick et al. (2014) and König et al. (2018); or under the permutation distribution, see Walther (2010).

## 5 The multivariate case

Surprisingly, the heuristics, methodology and optimality results described in the previous sections also apply in the multivariate setting, with no fundamentally different changes to the respective formulas if the scanning windows are sufficiently regular, e.g., balls or rectangles (even with variable aspect ratio). To appreciate this result, note that the heuristic behind the optimal detection threshold (8) is the well-known fact that the maximum of \( n \) i.i.d. standard normals concentrates around \( \sqrt{2 \log n} \). Now suppose we were to maximize over \( n^d \) rather than \( n \) independent normals, i.e., we massively increase the scale of the multiple testing problem. Since \( \sqrt{2 \log n^d} = \sqrt{(2d) \log n} \), one sees that the constant \( \sqrt{2} \) in the detection threshold (8) measures in a certain sense the difficulty of the detection problem and therefore plays a crucial role. This explains the effort to bound the constant in (8) as tightly as possible, in contrast to many other theoretical results in the statistics literature where constants typically play a minor role. In fact, due to its importance, Arias-Castro et al. (2005) call the constant \( d \) in the threshold \( \sqrt{(2d) \log n} \) the exponent of effective dimension.

At first sight, such a massive increase in the multiple testing problem is to be expected by scanning in \( d \)-dimensional rather than in univariate space. For example, there are of the order \( n^2 \) univariate intervals that contain distinct subsets of \( n \) points sampled from \( U[0, 1] \) (since there are \( n \) left endpoints and \( n \) right endpoints). In contrast, there are \( \sim n^{2d} \) axis-parallel rectangles that contain distinct subsets of \( n \) points sampled from \( U[0, 1]^d \). However, Arias-Castro et al. (2005) show, in the regression setting with \( n \times \ldots \times n = n^d \) observations on a regular \( d \)-dimensional grid, that for many relevant classes of scanning windows, such as axis-parallel rectangles and balls, the ‘effective dimensionality’ of the multiple testing problem is essentially linear in the sample size \( N = n^d \). That is, by showing that many of these scanning windows have a sizable overlap and are therefore highly correlated, they show that the scan (3) over all \( \sim n^{2d} \) windows behaves like the maximum of only \( \sim N = n^d \) independent normals. Walther (2010) gives a corresponding construction for \( N = n \) random design points in \( \mathbb{R}^d \), which likewise shows that scanning over all \( \sim n^{2d} \) axis-parallel rectangles that contain distinct subsets of the sample reduces to a problem that is essentially linear in the sample size \( N = n \) (so the reduction in the random design case is formally more pronounced than in the case of a regular grid with \( N = n^d \) observations). Arias-Castro et al. (2005) derive the detection threshold \( \mu = \mu(N, w) \geq (\sqrt{2} + \eta) \sqrt{\log N \log w} \) for any fixed \( \eta > 0 \), i.e., the exponent of effective dimension is at most 1. Walther (2010) shows that with the blocked scan it is in fact possible to attain the better threshold (8), i.e., one can replace \( \log N \) in the above threshold by \( \log \frac{N}{w} \). This means that for window sizes of, say, \( w = N^{-\frac{1}{2}} \), the exponent of effective dimension is in fact \( \frac{1}{2} \). Datta and Sen (2018) arrive at this result with the calibration (5).

A further advantage of using scale-dependent calibrations is that these calibrations allow to remove the ‘curse
of dimensionality': if the signal is supported on a lower-dimensional marginal, then the d-dimensional scan with a scale-dependent calibration has essentially the same detection power as an optimal lower-dimensional scan would have, so there is no fundamental additional price to pay for scanning in the higher-dimensional space, see Walther (2010) for details.

Other related results in the multivariate setting are given by Arias-Castro et al. (2011), who consider optimal detection when scanning over a network, while Datta and Sen (2018) and König et al. (2018) derive related results when the error distribution is a Brownian sheet on $[0,1]^d$ and an exponential family on a rectangular grid, respectively. Sharpnack and Arias-Castro (2016) derive the asymptotic null distributions for various calibrations of the scan over a d-dimensional grid.

As pointed out in Section 2.1, asymptotic optimality properties are typically not sufficient to ascertain a good performance of scanning methodology. This applies especially in the multivariate setting, where the massive multiple testing inherent in multivariate scanning may lead to a disappointing performance that is not adequately reflected by asymptotic performance guarantees, even for a large sample size. It is therefore advisable to evaluate and compare procedures with finite sample criteria, such as the realized exponent mentioned in Section 2.1, which measures how close the procedure comes to attaining the exponent of effective dimension described above. That is, the realized exponent is the finite sample counterpart to the asymptotic concept of the exponent of effective dimension, and it reflects the actual performance of a procedure in a given setting with a given sample size.

6 Computing the scan statistic

Evaluating the scan statistic, whether in its traditional form (2) or with any of the calibrations discussed above, requires to evaluate $\sum_{i=1}^k Y_i$ for $1 \leq j < k \leq n$. Thus a straightforward implementation results in a $O(n^2)$ algorithm, which makes the computation infeasible even for problems of moderate size. However, it turns out that it is possible to approximate the scan with sufficient precision using algorithms that have linear complexity, up to logarithmic terms. The key idea for a fast but accurate approximation is the observation that if one examines the interval $[j, k]$ where $j$ and $k$ are far apart, then not much is gained by also examining intervals with similar endpoints, such as $[j-1, k+1]$. Therefore, when examining large intervals, it suffices to consider endpoints on a coarse grid: If the grid spacing is small relative to the length of the interval, then the approximation error will be small. Shorter intervals require a finer grid spacing for a good approximation. This idea can be used to construct a collection of intervals that is rich enough to allow optimal detection (i.e. has small enough approximation error), while it is also sparse enough to allow fast computation (i.e. there should be no more than about $O(n \log n)$ intervals). The heuristic reason why this is possible is that the $O(n^2)$ complexity is largely due to the larger intervals, and it is precisely those that can be approximated well with a coarse grid, thus affording considerable savings.

In more detail, such a construction can be implemented with a dyadic decomposition of the interval length, so that intervals of roughly the same length (up to a factor of 2, or some other factor) will be evaluated with a certain grid spacing: At level $\ell$, we consider intervals $(j, k)$ with lengths $k - j \in [2^{\ell}, 2^{\ell+1})$ and endpoints $j, k$ on a grid with grid spacing $d_\ell = \lceil 2^{\ell}/\sqrt{2\log(en2^{-\ell})} \rceil$, see Walther (2010) for the general multivariate construction and Walther and Perry (2019) for the special case of the univariate regression setting (1). Similar approximation schemes have been used successfully in numerical analysis and related areas, see in particular Neill and Moore (2004), Arias-Castro et al. (2005) and Sharpnack and Arias-Castro (2016) in the context of scanning. However, the key feature of the above construction is the particular choice of the grid spacing $d_\ell$. Letting the grid spacing grow with this particular rate is important for achieving the detection boundary (8) for
all window widths $w$, while still allowing efficient computation. Moreover, in the case of the Bonferroni scan it is imperative to choose the grid spacing $d_\ell$ in just the right way, as too many intervals would result in too large a Bonferroni correction that diminishes detection power. It is remarkable that such a construction exists which is both rich enough for optimal detection and also sparse enough for efficient computation as well as for achieving optimal detection with a simple Bonferroni correction. Thus this construction is closely connected to fundamental aspects of the theory behind scanning.

Fast computation with $O(n \log n)$ algorithms makes it possible to obtain critical values by simulation rather than by analytical derivation of the distribution of maxima such as (2), which requires sophisticated theoretical work, see e.g. Siegmund (1986), Loader (1991), Siegmund and Venkatraman (1995), Kabluchko (2011) or Sharpnack and Arias-Castro (2016). In particular, the use of size-dependent critical values has been greatly facilitated by the availability of these fast algorithms.

Finally, the above results extend to the multivariate setting. That is, there are suitable approximating sets for the collection of all axis-parallel rectangles (or other common geometric objects) that have a cardinality that is linear in the sample size, up to logarithmic terms. This was shown for the regression setting with $N = n^d$ observations on a $n \times \ldots \times n$ lattice in $\mathbb{R}^d$ by Arias-Castro et al. (2005), and for the density setting with $N = n$ observations by Walther (2010). The heuristic behind this result is that, just as $\frac{N}{w}$ disjoint intervals of length $w$ are required to cover the univariate lattice $\{1, \ldots, N\}$, one needs $\frac{N}{w}$ disjoint squares of area $w$ to cover a two-dimensional lattice of area $N$. Moreover, allowing axis-parallel rectangles rather than squares will result only in additional logarithmic factors: A square with side length $a$ can be used as a basis to approximate rectangles with the same area and the same left endpoint by considering the set of rectangles with sides $m^k a$ and $m^{-k} a$ for $k = 0, \pm 1, \pm 2, \ldots$ and some $m > 1$. Due to the geometric progression of the aspect ratio, a logarithmic number of indices $k$ will suffice for a good approximation, just as the simultaneous consideration of all windows sizes $w$ resulted in only a logarithmic factor due to dyadic decomposition of the window sizes.

References

Arias-Castro, E., Candès, E. J., and Durand, A. (2011). Detection of an anomalous cluster in a network. *Ann. Statist.* 39, 278–304.

Arias-Castro, E., Castro, R.M., Tánczos, E. and Wang, M. (2018). Distribution-free detection of structured anomalies: Permutation and rank-based scans. *J. Amer. Statist. Assoc.* 113, 789–801.

Arias-Castro, E., Donoho, D. and Huo, X. (2005). Near-optimal detection of geometric objects by fast multi-scale methods. *IEEE Trans. Inform. Theory* 51, 2402–2425.

Chan, H.P. (2009). Detection of spatial clustering with average likelihood ratio test statistics. *Ann. Statist.* 37, 3985–4010.

Chan, H.P. and Walther, G. (2013). Detection with the scan and the average likelihood ratio. *Statistica Sinica* 23, 409–428.

Cressie, N. (1977). On some properties of the scan statistic on the circle and the line. *J. Appl. Prob.* 14, 272–283.

Datta, P. and Sen, B. (2018). Optimal inference with a multidimensional multiscale statistic. [arXiv:1806.02194]
Dümbgen, L. and Spokoiny, V.G. (2001). Multiscale testing of qualitative hypotheses. *Ann. Statist.* 29, 124–152.

Dümbgen, L. and Walther, G. (2008). Multiscale inference about a density. *Ann. Statist.* 36, 1758–1785.

Frick, K., Munk, A. and Sieling, H. (2014). Multiscale change point inference. *J. R. Stat. Soc. Ser. B.* 76, 495–580.

Glaz, J., Naus, J. and Wallenstein, S. *Scan Statistics.* Springer Series in Statistics. Springer-Verlag, New York, 2001.

Kabluchko, Z. (2011). Extremes of the standardized gaussian noise. *Stochastic Processes and their Applications* 121, 515–533.

König, C., Munk, A. and Werner, F. (2018). Multidimensional multiscale scanning in exponential families: Limit theory and statistical consequences. [arXiv:1802.07995](https://arxiv.org/abs/1802.07995)

Kulldorff, M. (1997). A spatial scan statistic. *Commun. Statist. Th. Meth.* 26, 1481–1496.

Leadbetter, M. R., Lindgren, G. and Rootzén, H. *Extremes and related properties of random sequences and processes.* Springer Series in Statistics. Springer-Verlag, New York, 1983.

Loader, C. R. (1991). Large-deviation approximations to the distribution of the scan statistics. *Adv. Appl. Prob.* 23, 751–771.

Nagarwalla, N. (1996). A scan statistic with a variable window. *Statistics in Medicine* 15, 845–850.

Naus, J. I. and Wallenstein, S. (2004). Multiple window and cluster size scan procedures. *Meth. Comp. Appl. Probab.* 6, 389–400.

Neill, D. and Moore, A. (2004). A fast multi-resolution method for detection of significant spatial disease clusters. *Adv. Neur. Info. Proc. Sys.* 10, 651–658.

Neill, D.B. (2009). An empirical comparison of spatial scan statistics for outbreak detection. Internat. *Journal of Health Geographics* 8, 1–16.

Rivera, C. and Walther, G. (2013). Optimal detection of a jump in the intensity of a Poisson process or in a density with likelihood ratio statistics. *Scand. J. Stat.* 40, 752-769.

Rufibach, K. and Walther, G. (2010). The block criterion for multiscale inference about a density, with applications to other multiscale problems. *J. Comp. Graph. Statist.* 19, 175–190.

Sharpnack, J, and Arias-Castro, E. (2016). Exact asymptotics for the scan statistic and fast alternatives. *Elect. J. Statist.* 10, 2641-2684.

Siegmund, D. (1986). Boundary crossing probabilities and statistical applications. *Ann. Statist.* 14, 361–404.

Siegmund, D. and Venkatraman, E.S. (1995). Using the generalized likelihood ratio statistic for sequential detection of a change-point. *Ann. Statist.* 23, 255–271.
Walther, G. (2010). Optimal and fast detection of spatial clusters with scan statistics. *Ann. Statist.* **38**, 1010–1033.

Walther, G. and Perry, A. (2019). Calibrating the scan statistic: finite sample performance vs. asymptotics. [arXiv:2008.06136](https://arxiv.org/abs/2008.06136)

Walther, G. (2021). Tail bounds for empirically standardized sums. [arXiv:2109.06371](https://arxiv.org/abs/2109.06371)