Satellite conjunction assessment: Statistical space oddity?

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Satellite conjunctions involving ‘near misses’ of space objects are becoming increasingly likely. One approach to risk analysis for them involves the computation of the collision probability, but this has been regarded as having some counter-intuitive properties, and its meaning as a probability is unclear. We formulate an alternative approach based on a simple statistical model that allows highly accurate inference on the miss distance between the two objects, show that this provides a close approximation to a default Bayesian approach, illustrate the method with a case study, and give Monte Carlo results to show its excellent performance.

I. Introduction

The expansion of the aerospace industry and the increasing number of space objects, especially in Low Earth Orbit where most spacecraft operate, means that risk assessment and collision avoidance manoeuvres are vital to ensure the safety of spacecraft. A great deal of effort has been put into conjunction assessment for orbiting objects, generally by estimating the probability of collision between two space objects [1]. This probability is calculated at the time of the closest approach using the estimated position and velocity vectors for the two objects and the associated error covariances and, in a short-term conjunction, is an integral of a two-dimensional Gaussian probability density function over the collision cross-sectional area. Although unavailable in explicit form, it can readily be evaluated numerically [2–6]. However both more precise and less precise measurement reduce the collision probability, a ‘dilution’ property that has been seen as paradoxical and its interpretation is not clear-cut [7]. Another important criterion for risk assessment is the closest approach distance, or miss distance, as a miss distance that is likely to be lower than a specified safety threshold indicates a situation that requires action. There are many algorithms to compute the minimum distance allowed by the geometry of the problem, often as the root of a polynomial equation [8–10].

In this work, we formulate a statistical model for conjunction assessment that resolves the apparent difficulties with the collision probability and suggests that the miss distance is a more appropriate focus of interest. We discuss inference for this distance based on standard likelihood theory [11, chapter 9], and also describe an improved theory that is highly accurate and should give results very similar to a Bayesian formulation [12]. Our approach is based on significance functions [13] and provides both point and interval estimates for the miss distance, with the intervals containing the true miss distance with a specified probability under the model. We can also test whether the true distance is higher than the safety threshold, in order to guide decisions about avoidance manoeuvres [14].
The paper is organized as follows. In Section II we formulate the conjunction assessment problem in statistical terms and discuss the relationship between the conjunction probability and miss distance, also elucidating the so-called dilution paradox of the former. In Section III we introduce significance functions and discuss how they provide calibrated frequentist inference, present elements of modern likelihood inference and link them to the Bayesian approach. In Section IV we apply these ideas to the satellite conjunction problem and illustrate them with a case study. Section V contains a Monte Carlo study of the calibration, and Section VI discusses the use of several successive observations on a conjunction, decision analysis and conjunction geometry.

II. Conjunction assessment

A. Problem formulation

Modelling and analysis of the relative motion of two space objects has been successfully applied to many space missions [15]. Algebraic models for relative errors were proposed by Hill [16] and Clohessy and Wiltshire [17] and developed in Chen et al. [1]. Many authors [2–4, 6, 18] have considered the two objects as ellipsoids and attempted to estimate the probability that they will collide. As mentioned above, this probability has been considered by some to have paradoxical properties [7], but these evaporate when the problem is formulated using a statistical model, as we shall see. Recall that a parametric statistical model treats the available data \( y \) as the realisation of a random variable \( Y \) whose probability density function \( f(y; \theta) \) is determined by unknown parameters \( \theta \), and the goal is inference about the value of a parameter \( \psi = \psi(\theta) \) based on \( y \). Below we take \( \psi \) to be the miss distance and suppose that a collision occurs if the two objects pass within a minimum distance of each other, the combined hard-body radius, \( \psi_{\text{min}} \).

Suppose initially that the true current positions \( \mu_{s1} \) and \( \mu_{s2} \) and velocities \( v_{s1} \) and \( v_{s2} \) of the two objects have been observed; all these are \( 3 \times 1 \) vectors. Define \( \mu = \mu_{s2} - \mu_{s1} \) and \( v = v_{s2} - v_{s1}, \) so the second object is considered relative to an origin at the first object. In this frame of reference and if the relative motion is linear the second object traverses the line \( \mu + cv, \) where \( c \in \mathbb{R} \). Its distance from the first, \( (\mu + cv)^T(\mu + cv) \), is minimised by choosing \( c = -v^T\mu/v^Tv, \) at which point the minimum squared distance is \( \psi^2 = \mu^T\mu - (\mu^Tv)^2/v^Tv. \) In terms of spherical polar coordinates we can write

\[
\begin{align*}
\mu & = \|\mu\| (\sin \theta_1 \cos \phi_1, \sin \theta_1 \sin \phi_1, \cos \theta_1)^T, \\
v & = \|v\| (\sin \theta_2 \cos \phi_2, \sin \theta_2 \sin \phi_2, \cos \theta_2)^T,
\end{align*}
\]

where \( \| \cdot \| \) denotes the Euclidean norm and \( 0 \leq \theta_1, \theta_2 \leq \pi \) and \( 0 \leq \phi_1, \phi_2 < 2\pi \) are the polar and azimuthal angles for \( \mu, v. \) The minimum distance between the two objects, the miss distance, is

\[
\psi = \|\mu\|(1 - \cos^2 \beta)^{1/2} = \|\mu\| |\sin \beta|,
\]

\( \Box \)
where $\beta$, the angle between the location and velocity vectors $\mu$ and $\nu$, satisfies

$$\cos \beta = \sin \theta_1 \cos \phi_1 \sin \theta_2 \cos \phi_2 + \sin \theta_1 \sin \phi_1 \sin \theta_2 \sin \phi_2 + \cos \theta_1 \cos \theta_2. \quad (4)$$

When $\beta = 0$ we distinguish two cases: if $\mu^T \nu < 0$ the second object will pass through the origin, leading to a collision, whereas if $\mu^T \nu > 0$ the second object is heading away from the origin, so its current position is the closest it will come to the first object. More generally, $\psi < \|\mu\|$ only if $\cos \beta < 0$, i.e., $\pi/2 < \beta < 3\pi/2$. For $\mu$ and $\nu$ to be collinear but pointing in opposite directions we need $\phi_2 = \pi + \phi_1$ and $\theta_2 = \pi - \theta_1$, and then $\cos \beta = \cos(\theta_1 + \theta_2) = -1$, so $\beta = \pi$ and hence $\psi = 0$, as expected. To lighten the notation below we write $\lambda = (\theta_1, \phi_1, \|\nu\|, \theta_2, \phi_2)$, and $\vartheta = (\psi, \lambda)$.

In the above deterministic setting the collision probability $p_c \equiv p_c(\vartheta)$ takes two possible values,

$$p_c(\vartheta) = \begin{cases} 0, & \psi > \psi_{\text{min}}, \\ 1, & 0 \leq \psi \leq \psi_{\text{min}}, \end{cases} \quad (5)$$

and a decision-maker can make an ideal decision. In reality, of course, both $\mu$ and $\nu$ are observed with error, and we follow the literature and assume that the available observations on the positions and velocities of the two objects have a multivariate normal distribution with known covariance matrix. If so, then the vector $y$ containing the observed position and velocity of the second object relative to the first has a six-dimensional normal distribution, and we suppose that this has mean vector $\eta(\lambda) = (\mu(\psi, \lambda)^T, \nu(\lambda)^T)^T$ given by equations (1)–(4) and known $6 \times 6$ covariance matrix $\Omega^{-1}$; $\Omega$ is known as the dispersion matrix.

**B. Conjunction probability or miss distance?**

Two points are immediately clear from the above very simple statistical model for satellite conjunction.

First, the conventional target of inference here, the collision probability $\tilde{p}_c$, is a function of the parameters only. The two-dimensional probability of collision, $\tilde{p}_c$, which is calculated by numerical methods and used to guide decisions about satellite manoeuvres, depends on the data $y$ and the known covariance matrix, is therefore a statistical estimator of $p_c$. Hence the ‘paradoxical’ behaviour whereby $\tilde{p}_c$ is very tiny when $y$ has a very large variance and then increases when that variance decreases is the behaviour of an estimator, not of a parameter of the model. The estimator $\tilde{p}_c$ depends on the covariance matrix of $y$, and as the variance of $y$ decreases we expect that either $\tilde{p}_c \to 1$, if a collision will occur, or $\tilde{p}_c \to 0$, otherwise; in both cases $\tilde{p}_c \to p_c$, as we should expect when the data become noiseless. Thus probability dilution is the natural behaviour of an estimator that depends on the variability of the underlying data, not a paradox.

Second, the fact that $p_c$ takes just two values whereas the miss distance $\psi$ takes values in a continuum suggests that $\psi$ is a better overall target of inference. For example, a maximum likelihood estimator of $p_c$ would have the form $I(\tilde{\psi} \leq \psi_{\text{min}})$, where $I(\cdot)$ denotes the indicator function and $\tilde{\psi}$ the maximum likelihood estimator of $\psi$, and clearly $\tilde{\psi}$
more informative. Moreover in a Bayesian framework the unknown parameters would be regarded as random variables, the model above would be complemented by a prior density, and the posterior probability of collision given the data would be $\Pr(\psi \leq \psi_{\text{min}} \mid y)$, obtained by integrating the posterior density of $\psi$ given $y$. In this setting too the collision probability is based on knowledge about the miss distance $\psi$, suggesting that the latter is the more fundamental quantity.

In Section III.D we discuss Bayesian inference in more detail, and in Section IV we show how inference on $\psi$ provides a significance probability whose interpretation is similar to that of $\hat{p}_c$.

Motivated by these considerations, we turn to inference on $\psi$ based on the observed value $y^o$ of $y$. If the data suggest that $\psi$ is lower than a safety threshold $\psi_0$, possibly with $\psi_0 > \psi_{\text{min}}$ for a safety margin, then action to avert a collision should be considered. Our goal below is therefore inference on the unknown miss distance $\psi$, allowing for the fact that $\lambda = (\theta_1, \phi_1, ||v||, \theta_2, \phi_2)$ is also unknown and must be estimated; we can write the relative distance vector using (1) but with $||\mu||$ replaced by $\psi/|\sin \beta|$, for $\beta \neq \pi$. With this setup $\psi$ and $\lambda$ are variation independent, as required in Section III.C see Appendix B.

We return to this model after outlining elements of the theory of inference.

### III. Inference

#### A. Calibration and significance functions

Statistical inference involves statements about the properties of a probability distribution that is assumed to have given rise to observed data $y^o$. In the simplest parametric setting the property of interest is a scalar parameter $\psi$ and the likelihood function $L(\psi) = f(y^o; \psi)$ is used to compare the plausibility of different values of $\psi$ as explanations for $y^o$. The best-fitting model is provided by the maximum likelihood estimate based on $y^o$, $\hat{\psi}^o$, and the relative likelihood $RL(\psi) = L(\psi)/L(\hat{\psi}^o)$, which has maximum value 1, allows values of $\psi$ to be compared. A ‘pure likelihood’ approach [19] treats any $\psi$ for which $RL(\psi) \geq c$ as plausible, but with $c$ chosen essentially arbitrarily. In practice further information is typically incorporated to avoid the subjectivity of this approach.

Bayesian inference treats $\psi$ as a random variable and entails choosing a density $\pi(\psi)$ that weights values of $\psi$ according to their prior plausibility. This is updated in light of $y^o$ using Bayes’ formula, resulting in the posterior distribution function

$$\Pr(\psi \leq \psi_0 \mid y^o) = \frac{\int_{-\infty}^{\psi_0} L(\psi)\pi(\psi)\,d\psi}{\int_{-\infty}^{\infty} L(\psi)\pi(\psi)\,d\psi}. \tag{6}$$

The main difficulty here is the choice of $\pi$: subjective priors are often used, and if these are badly chosen then (6) may have poor properties when used repeatedly. When the potential losses due to actions that might be taken in light of knowledge about $\psi$ can be measured, the data can be used to choose the action that minimises the expected loss taken with respect to the posterior distribution of $\psi$; see Section VI.C.

Frequentist approaches to calibrating the likelihood are often regarded as preferable. They treat the observed data as
the outcome from a random experiment, hypothetical repetition of which provides a basis for inference [14]. In the simplest possible case \( \tilde{\psi}^o \) is regarded as a realization of a random variable \( \tilde{\psi} \) that has a normal distribution, \( \mathcal{N}(\psi, \lambda^2) \), under repeated sampling, with \( \lambda \) known. This implies that

\[
\Pr(\tilde{\psi} \leq \tilde{\psi}^o; \psi) = \Phi\left\{ (\tilde{\psi}^o - \psi) / \lambda \right\},
\]

(7)

where \( \Phi \) denotes the standard normal cumulative distribution function. The significance function [7], also called the confidence distribution or P-value function [20–22], is then the basis of inference on \( \psi \). For example, the null hypothesis that \( \psi = \psi_0 \) can be tested against the alternative that \( \psi > \psi_0 \) by computing the significance probability

\[
p_{\text{obs}} = \Pr(\tilde{\psi} \geq \tilde{\psi}^o; \psi_0),
\]

(8)

small values of which are regarded as evidence against the null hypothesis in favour of the alternative; here \( p_{\text{obs}} = 1 - \Phi\left\{ (\tilde{\psi}^o - \psi_0) / \lambda \right\} \). Likewise a two-sided \( (1 - 2\alpha) \times 100\% \) confidence interval for the value of \( \psi \) underlying the data, the so-called ‘true value’, has as its upper and lower limits \( U_\alpha \) and \( L_\alpha \) the solutions to the equations

\[
\Pr(\tilde{\psi} \leq \tilde{\psi}^o; U_\alpha) = \alpha, \quad \Pr(\tilde{\psi} \leq \tilde{\psi}^o; L_\alpha) = 1 - \alpha,
\]

and this yields \( I_{1-2\alpha} = (L_\alpha, U_\alpha) = (\tilde{\psi}^o - \lambda z_{1-\alpha}, \tilde{\psi}^o - \lambda z_\alpha) \), where \( z_p \), the \( p \) quantile of the standard normal distribution, satisfies \( \Phi(z_p) = p \) for \( 0 < p < 1 \). The limits of \( I_{1-2\alpha} \) simplify to the familiar \( \tilde{\psi}^o \pm \lambda z_{1-\alpha} \) on recalling that \( z_{1-\alpha} = -z_\alpha > 0 \). In this ideal case the inferences are perfectly calibrated: under repeated sampling with \( \psi = \psi_0 \) the significance probability \( p_{\text{obs}} \) has an exact uniform distribution and \( I_{1-2\alpha} \) contains the true value of \( \psi \) with probability exactly \( 1 - 2\alpha \), for any \( \alpha \in (0, 0.5) \). When \( \psi = \psi_0 \), therefore, there is a probability \( p_{\text{obs}} \) that a decision to reject this hypothesis in favor of the alternative based on a significance probability \( p_{\text{obs}} \) will be incorrect.

Significance functions are decreasing in the parameter and have the properties of survivor functions, so the confidence density based on differentiating (7),

\[
- \frac{\partial \Pr(\tilde{\psi} \leq \tilde{\psi}^o; \psi)}{\partial \psi}, \quad \psi > 0,
\]

(9)

has the formal properties of a probability density function for \( \psi \). The confidence density and its integral, the confidence distribution, can be regarded as frequentist summaries of the information about \( \psi \) based on the observed data; see Schweder and Hjort [22]. Unlike the posterior density obtained from (6), no prior information is involved, and despite the use of the word ‘density’ for (9), \( \psi \) is regarded as an unknown constant.
B. Approximate inference

In Section III.A, \( \hat{\psi} \) was assumed to have an exact normal distribution, but the argument often applies approximately when some measure of precision, typically the sample size \( n \), becomes large. Under mild regularity conditions the maximum likelihood estimator \( \hat{\psi} \) has an approximate normal distribution centered at the true parameter \( \psi \) with variance \( 1/j(\hat{\psi}) \), where \( j(\hat{\psi}) = \partial^2 \log L(\hat{\psi})/\partial \psi^2 \) is the observed information. This allows indirect calibration of \( \psi \) using the Wald statistic

\[
\tilde{w}(\psi) = j(\hat{\psi})^{1/2}(\hat{\psi} - \psi),
\]

corresponding to a quadratic approximation to \( \log RL(\psi) \), and direct calibration using the likelihood root

\[
\tilde{r}(\psi) = \text{sign}(\hat{\psi} - \psi)[2 \log RL(\psi)]^{1/2}.
\]

Both \( \tilde{w}(\psi) \) and \( \tilde{r}(\psi) \) are approximate pivots: they are functions of the data and parameter and have approximate standard normal distributions if \( \psi \) equals its true value. The approximations introduce so-called first-order error, of size \( O(n^{-1/2}) \), in (7). For more details, see, for example, Chapter 9 of Cox and Hinkley [11].

To illustrate these approximations, consider a single observation from the Rayleigh distribution, which arises as the length \( y \) of a bivariate normal vector whose components are independent \( N(0, \psi^2) \) variables. The probability density function for \( y \) is

\[
f(y; \psi) = \frac{y}{\psi^2} e^{-y^2/(2\psi^2)}, \quad y > 0, \quad \psi > 0,
\]

and one can readily check that \( \hat{\psi} = y/\sqrt{2}, j(\hat{\psi}) = 4/\hat{\psi}^2 \) and

\[
\tilde{w}(\psi) = 2(1 - \psi/\hat{\psi}), \quad \tilde{r}(\psi) = \text{sign}(\hat{\psi} - \psi)[2 \{2 \log(\psi/\hat{\psi}) + (\hat{\psi}/\psi)^2 - 1\}]^{1/2}.
\]

The left-hand panel of Fig 1 shows the significance functions \( \Phi \{w^o(\psi)\} \) and \( \Phi \{r^o(\psi)\} \) when \( y^o = \sqrt{2} \), so \( \hat{\psi} \) has observed value \( \hat{\psi}^o = 1 \). The functions are decreasing in \( \psi \) and the maximum likelihood estimate and the limits of the 90% confidence interval are the values of \( \psi \) for which the functions equal 0.5 and 0.05, 0.95, respectively. Evidence against the null hypothesis \( \psi = \psi_0 = 0.3 \) in favor of the alternative \( \psi > \psi_0 \) is found from the P-value \( \{8\} \) given by the intersections of the significance functions with the vertical line \( \psi = 0.3 \); for the Wald statistic we obtain \( 1 - \Phi \{w^o(\psi_0)\} = 0.0808 \) and for the likelihood root we obtain \( 1 - \Phi \{r^o(\psi_0)\} = 4.33 \times 10^{-5} \). If a test was performed at the 5% or even at the 0.01% levels, different decisions about the null hypothesis would be taken, depending on which of these functions was used. The right-hand panel of Fig 1 shows \( w^o(\psi) \) and \( r^o(\psi) \) directly, from which it is easier to read off confidence intervals.

In the Rayleigh example \( \hat{\psi}/\psi \) has a known distribution, so the left-hand side of (7) provides an exact significance
Fig. 1 Rayleigh example. Left: significance functions based on likelihood root $r^0(\psi)$ (solid black), Wald statistic $w(\psi)$ (dotted blue), exact (wide cyan) and modified likelihood root $r^{*0}(\psi)$ (red dashes). The horizontal lines at 0.95, 0.05 provide limits for a 90% confidence interval, and that at 0.5 intersects with $w^0(\psi)$ and $r^0(\psi)$ at the maximum likelihood estimate $\hat{\psi}^0 = 1$. The vertical line at $\psi_0 = 3$ allows calculation of the significance probability for testing $\psi = \psi_0$ against the hypothesis that $\psi < \psi_0$. Right: the same quantities transformed to the standard normal scale.

function. The sample size here is $n = 1$, so it is no surprise that the exact function differs greatly from the large-sample approximations based on $w^0(\psi)$ or $r^0(\psi)$; it gives an exact significance probability of $1.49 \times 10^{-5}$ for testing $\psi_0 = 3$. Remarkably, however, an approximation that treats the modified likelihood root

$$r^*(\psi) = r(\psi) + \frac{1}{r(\psi)} \log \left( \frac{q(\psi)}{r(\psi)} \right)$$

(10)

as standard normal is essentially exact; its significance probability is $1.55 \times 10^{-5}$, giving a relative error of 3.6%. The approximation based on $r^*(\psi)$ is said to be third-order accurate, i.e., its error is $O(n^{-3/2})$, and moreover this error is relative, so high accuracy can be expected even when the true probabilities are small. Here $n = 1$, so the approximation yields quasi-perfect calibration of different values of $\psi$. In this particular example $q(\psi) = 1 - \hat{\psi}^2/\psi^2$; we discuss its general construction in Appendix A.

C. Several parameters

Models with a single scalar parameter are unusual: other parameters are usually present and must be estimated. Despite this, near-exact inferences remain possible in many cases, as we now outline.

Suppose that the density function $f(y; \theta)$ now depends on an unknown $d$-dimensional parameter $\theta$, which comprises
a scalar interest parameter $\psi$ that is the focus of the investigation and a nuisance parameter $\lambda$ that is needed for realistic modeling but whose value is of secondary concern; $\psi$ and $\lambda$ are supposed to be variation independent. As $\lambda$ is unknown, it must be replaced by an estimate, and we see from (7) that this would introduce errors.

In this situation a natural analogue of the relative likelihood is the profile relative likelihood function, \( RL_p(\psi) = \frac{L(\hat{\theta}^o)}{L(\hat{\theta}_\psi^o)} \), where the maximum likelihood estimate $\hat{\theta}^o = (\hat{\psi}^o, \hat{\lambda}^o)$ maximises the log-likelihood $\ell(\theta) = \log f(y^o; \theta)$ with respect to $\theta$, and the partial maximum likelihood estimate $\hat{\theta}_\psi^o = (\psi, \hat{\lambda}_\psi^o)$ maximizes $\ell(\theta)$ with respect to $\lambda$ for fixed $\psi$. The large-sample properties of the maximum likelihood estimator $\hat{\theta}$ under repeated sampling are well-known \[11, Chapter 9\]: as the sample size $n \to \infty$ and under mild regularity conditions, $\hat{\theta}$ has an approximate $d$-dimensional normal distribution with mean the true parameter $\theta$ and covariance matrix $\mathbf{\Theta}$, where $\mathbf{\Theta} = \frac{\partial^2 \ell(\theta)}{\partial \theta \partial \theta^T}$ is the observed information matrix and $\theta^T$ is the transpose of the $d \times 1$ vector $\theta$. Under these conditions the error committed by replacing parameters in (7) by their estimates is $O(n^{-1/2})$, giving first-order approximations, and the same error is committed by treating the likelihood root

\[ r(\psi) = \text{sign}(\hat{\psi} - \psi) \left\{ 2 \log RL_p(\psi) \right\}^{1/2} \] (11)

or the Wald statistic

\[ w(\psi) = J_p(\hat{\psi})^{1/2}(\hat{\psi} - \psi), \] (12)

as standard normal; here

\[ J_p(\psi) = \begin{vmatrix} j \left( \hat{\theta}_\psi \right) \end{vmatrix} \begin{vmatrix} J_{,11} \left( \hat{\theta}_\psi \right) \end{vmatrix}, \]

$| \cdot |$ indicates the determinant, and $J_{,11}(\theta)$ is the ($\lambda, \lambda$) corner of $j(\theta)$. The improvement to third-order accuracy seen in the scalar case is again given by \[10\], now using \[11\] and

\[ q(\psi) = \begin{vmatrix} \varphi(\hat{\theta}) - \varphi(\hat{\theta}_\psi) \varphi_{,1}(\hat{\theta}_\psi) \end{vmatrix} \begin{vmatrix} J(\hat{\theta}) \end{vmatrix}^{1/2} \begin{vmatrix} J_{,11}(\hat{\theta}_\psi) \end{vmatrix}^{1/2}. \] (13)

Here $\varphi(\theta)$ is a $d \times 1$ constructed parameter that can be viewed as a directional derivative of the log-likelihood, and $\varphi_{,1}(\theta) = \partial \varphi(\theta) / \partial \theta^T$ and $\varphi_{,11}(\theta) = \partial \varphi(\theta) / \partial \lambda^T$ are respectively $d \times d$ and $d \times (d - 1)$ matrices; see Appendix A.

In applications, expressions (11)–(13) are evaluated at the observed data $y^o$ and the corresponding estimates $\hat{\theta}^o$ and $\hat{\theta}_\psi^o$, leading to the approximate significance function

\[ \Pr(\hat{\theta} \leq \hat{\psi}^o; \psi) = \Phi \{ r^{\psi o}(\psi) \} \left\{ 1 + O(n^{-3/2}) \right\}, \] (14)

\[ \text{8} \]
which can be used in the same way as (7).

D. Bayesian approximation

In the setting with several parameters, expression (6) generalizes to the marginal posterior distribution of the scalar interest parameter \( \psi \), i.e.,

\[
\Pr(\psi \leq \psi_0 \mid y^0) = \frac{\int_{-\infty}^{\psi_0} \int L(\psi, \lambda) \pi(\psi, \lambda) \, d\lambda \, d\psi}{\int_{-\infty}^{\infty} \int L(\psi, \lambda) \pi(\psi, \lambda) \, d\lambda \, d\psi},
\]

where \( \pi(\psi, \lambda) \) is the prior density. On approximating both integrals using Laplace’s method, it turns out that (12, Section 8.7)

\[
\Pr(\psi \leq \psi_0 \mid y^0) = \Phi \left( r^o_B(\psi_0) \right) \left( 1 + O(n^{-1}) \right),
\]

where \( r^o_B(\psi) \) is defined by equation (10) but with \( q^o(\psi) \) replaced by

\[
q^o_B(\psi) = \frac{df(\hat{\theta}_\psi)}{d\psi} \times \frac{|J_{LL}(\hat{\theta}_\psi)|^{1/2}}{|J(\hat{\theta})|^{1/2}} \times \frac{\pi(\hat{\theta})}{\pi(\hat{\theta}_\psi)}
\]

evaluated at the observed data \( y = y^0 \) and the corresponding estimates \( \hat{\theta} = \hat{\theta}^o \) and \( \hat{\theta}_\psi = \hat{\theta}^o_\psi \). Thus there is a close parallel between frequentist and the Bayesian approximations and, with an appropriate choice of the prior \( \pi \), the probabilities that the corresponding confidence intervals contain \( \psi_0 \) differ by only \( O(n^{-1}) \). In the present case the Jeffreys prior, which gives inferences invariant to 1–1 transformation of \( \theta \), is \( |\eta_\theta(\theta)| \), though this prior is criticised by Fraser et al. [23]. Further details can be found in Appendix D.

In a similar context Davison and Sartori [24] compare the performances of \( r^o_B(\psi) \) and of \( r^{*o}(\psi) \) and find that the former performs rather worse. The Bayesian confidence intervals are slightly shorter and tend to contain the true parameter less often. Although the parallel is close and the results similar, we do not implement Bayesian approximations in the present setting; rather we find it reassuring that Bayesian and frequentist inferences can be shown to agree closely. If reliable prior information was available on each likely conjunction, then a Bayesian approach would be indicated.

IV. Inference for conjunction assessment

A. Likelihood

In this section we apply the standard theory described in Section III.C to the statistical model described in Section II. As mentioned there, the likelihood function plays a central role. After dropping irrelevant additive constants, the log-likelihood function is

\[
\ell(\theta) = -\frac{1}{2} \{y - \eta(\theta)\}^T \Omega \{y - \eta(\theta)\},
\]
where $\mathbf{\theta} = (\psi, \lambda)$ contains the miss distance $\psi$ for which inference is required and the five-dimensional nuisance parameter vector $\lambda = (\theta_1, \phi_1, \|v\|, \theta_2, \phi_2)$. The maximum likelihood estimator $\hat{\mathbf{\theta}}$ based on the observed relative distance and velocity contained in the $6 \times 1$ vector $y$ satisfies $\eta(\hat{\mathbf{\theta}}) = y$ and the observed information matrix is

$$j(\hat{\mathbf{\theta}}) = \frac{\partial \eta^T(\mathbf{\theta})}{\partial \mathbf{\theta}} \frac{\partial \eta(\mathbf{\theta})}{\partial \mathbf{\theta}^T} \bigg|_{\mathbf{\theta} = \hat{\mathbf{\theta}}},$$

where $\frac{\partial \eta^T(\mathbf{\theta})}{\partial \mathbf{\theta}}$ is a $6 \times 6$ matrix, and $\log RL_p(\psi) = -\ell(\hat{\theta}_p)$, where $\hat{\theta} = (\psi, \hat{\lambda})$ maximises $\ell(\mathbf{\theta})$ for fixed $\psi$. These quantities allow inference on $\psi$ based on the likelihood root \textsuperscript{[11]} and the Wald statistic \textsuperscript{[12]}, while the more accurate modified likelihood root \textsuperscript{[10]} also requires \textsuperscript{[13]}. The normal model is a curved exponential family \textsuperscript{[25, Section 5.2]} in terms of $\mathbf{\theta}$, so we can take $\varphi(\mathbf{\theta}) = \eta(\mathbf{\theta})$, the computation of $r^*(\psi)$ only involves $\eta(\mathbf{\theta})$ and its derivatives, and expression \textsuperscript{[13]} simplifies to

$$|\eta(\hat{\mathbf{\theta}}) - \eta(\hat{\mathbf{\theta}}_p)| \times |\Omega|^{1/2} \times |J_{\lambda\lambda}(\hat{\mathbf{\theta}}_p)|^{-1/2}. \quad (18)$$

Appendices C, D, and E contain the detailed calculations for this, for the Bayesian approximation, and numerical details.

Here there are six parameters and a single six-dimensional observation $y$, so the sample size is $n = 1$, and it appears that we cannot expect large-sample approximations to apply. However the covariance matrix for an average of $n$ independent observations would be $(n\Omega)^{-1}$, so a large sample size $n$ is equivalent to a small variance for the observations or equivalently large $\Omega$, which is the correct gauge of accuracy.

We express the role of the safety threshold $\psi_0$ in terms of a test of the null hypothesis $H_0 : \psi = \psi_0$ against the alternative hypothesis $H_+ : \psi > \psi_0$, with evasive action to be considered if the significance probability \textsuperscript{[8]} exceeds some threshold $\epsilon$, i.e., $H_0$ cannot be rejected at level $\epsilon$. The calibration of \textsuperscript{[8]} implies that if the true miss distance was $\psi_0$, then the false positive probability, that of considering action unnecessarily, would $1 - \epsilon$, whatever $\epsilon$ is chosen, though typically $\epsilon = 10^{-4}$ in practice. The choice of $H_+$ as alternative hypothesis ensures that $p_{\text{obs}}$ is small when both the estimated conjunction probability $\hat{p}_c$ and the Bayesian posterior probability $\Pr(\psi \leq \psi_0 | y)$ would also be small, notwithstanding their different interpretations. Hejduk et al. \textsuperscript{[26]} argue that the null hypothesis $\psi \leq \psi_0$ is unnatural, since it implies that the default ‘null’ situation is to anticipate a collision, but it appears more important to us that small values of $p_{\text{obs}}$ correspond to small conjunction probabilities, and this is ensured by the setup described above.

**B. Case study**

We illustrate the discussion above using the 10 February 2009 collision of the U.S. operational communications satellite Iridium 33 and the decommissioned Russian communications satellite Cosmos 2251. Table\textsuperscript{[1]} shows their positions and velocities at the time of the closest approach, and Table\textsuperscript{[2]} shows their relative position and velocity in Cartesian and spherical coordinates.

Figure\textsuperscript{[2]} shows the significance functions for this conjunction. The safety threshold of 650m, corresponding to
Table 1  Position and velocity coordinates of the U.S. and Russian satellites in the Cartesian system [1, Chapter 5].

| Object | Primary          | Secondary         |
|--------|------------------|-------------------|
| X (km) | 1457.273246      | 1457.532155       |
| Y (km) | 1589.568484      | 1588.932671       |
| Z (km) | 6814.189959      | 6814.316188       |
| V_x (km/s) | -7.001731       | 3.578705          |
| V_y (km/s) | 2.439512         | 6.172896          |
| V_z (km/s) | 0.926209         | 2.200215          |

Table 2  Conjunction geometry of the U.S. and Russian satellite collision event

| Conjunction geometry | Value       |
|----------------------|-------------|
| Miss distance (km)   | 0.698011    |
| ΔX (km)              | -0.258909   |
| ΔY (km)              | -0.635813   |
| ΔZ (km)              | 0.126229    |
| ΔV_x (km/s)          | 10.580436   |
| ΔV_y (km/s)          | -3.733384   |
| ΔV_z (km/s)          | 3.126424    |
| θ_1 (°)              | 1.3889      |
| θ_2 (°)              | 1.2990      |
| φ_1 (°)              | 1.9575      |
| φ_2 (°)              | -0.3392     |

ϕ_0 = 0.65, is very close to the estimated miss distance ϕ̂ = 0.698, so evasive action would be essential. In this situation the significance functions all lead to the same conclusion, indeed, those for the Wald statistic and the likelihood root are indistinguishable, but that for the modified likelihood root is shifted slightly to the left, slightly weakening any evidence that the true miss distance is greater than ϕ_0. The significance probabilities for testing ψ = ϕ_0 = 0.65 against H_+ : ψ > ϕ_0 are 0.415 for the Wald statistic and likelihood root, and 0.481 for the modified likelihood root, so the same conclusions would be drawn for both approaches, but clearly there is potential for different conclusions in some cases. The posterior probability Pr(ϕ ≤ ϕ_0 | ϕ) would be similar to the significance probability for the modified likelihood root, i.e., very close to 0.5.

V. Numerical results

A. General

Below we investigate the accuracy of the normal approximation to the Wald statistic, the likelihood root and the modified likelihood root in two scenarios. We do so in terms of one-sided error rates for confidence intervals (L_α, U_α)
for the true miss distance $\psi_0$ and use $Pr_0$ to indicate probability computed when $\psi = \psi_0$. An ideal two-sided equi-tailed confidence interval with coverage probability $1 - 2\alpha$ should satisfy $Pr_0(L_\alpha \leq \psi_0 \leq U_\alpha) = 1 - 2\alpha$ and have one-sided error rates $Pr_0(\psi_0 < L_\alpha)$ and $Pr_0(U_\alpha < \psi_0)$ both equal to $\alpha$; the error rates are also known as non-coverage probabilities. Departures from these error rates will indicate deficiencies of the confidence intervals and the corresponding tests, whereas close agreement will indicate that the inferences are well-calibrated.

The form of the covariance matrix used in practice depends on the type of the conjunction, which may be short-term or long-term [1, Chapter 5]. In a short-term conjunction, uncertainty on the velocity is negligible compared to uncertainty on the position. In a long-term conjunction, the motion is nonlinear and a more complicated model is needed to compute the covariance matrix. In both cases, the quality of the risk assessment depends heavily on the covariance matrix. Below we suppose that the error covariance matrix for the relative distance and velocity of the second satellite relative to the first is given by

$$
\Omega^{-1} = \begin{bmatrix}
P_1 & P_{12} \\
P_{12} & P_2
\end{bmatrix},
$$

where $P_1$, $P_2$, and $P_{12}$ are the position, the velocity and the cross-correlation covariance matrices, respectively. We assume that $P_{12} = 0_{3x3}$, and choose $P_1 = \tau \sigma^2 I_3$ and $P_2 = \sigma^2 I_3$. This choice implies that the standard deviation

\[\text{Fig. 2} \quad \text{Significance functions for the U.S. and Russian satellite collision event. Left: significance functions based on likelihood root } r^\theta(\psi) \text{ (solid black), Wald statistic } w(\psi) \text{ (blue dots), and modified likelihood root } r^{*\theta}(\psi) \text{ (red dashes). The horizontal lines at } 0.95, 0.05 \text{ provide limits for a } 90\% \text{ confidence interval, and that at } 0.5 \text{ intersects with } w^\theta(\psi) \text{ and } r^\theta(\psi) \text{ at the maximum likelihood estimate } \hat{\psi} = 0.698. \text{ The dashed vertical line at } \psi_0 = 0.65 \text{ allows calculation of the significance probability for testing } \psi = \psi_0 \text{ against the hypothesis that } \psi < \psi_0. \text{ Right: the same quantities transformed to the standard normal scale.}\]
of position errors along each axis direction is $\sqrt{\tau} \sigma$ (km) and the standard deviation of velocity errors is $\sigma$ (km/s). Uncertainty on the position is typically larger than that on the velocity, and then $\tau > 1$.

### B. Scenario 1

In our first setting the relative distance, relative velocity and spherical coordinates of two satellites are as given in Table 3. The relative distance is around 102 km and the relative speed around 11.7 km/s, the value of $\sigma^2$ varies over the range $10^{-3}$ to 2, and that of $\tau$ varies from 1 to 3.

Table 4 show the error rates for the Wald statistic, the likelihood root $r$ and the modified likelihood root $r^*$ based on 10,000 simulated datasets generated using various combinations of values of $\sigma$ and $\tau$. For very small $\sigma^2$ all three sets of error rates are close to the nominal values, but problems with the Wald statistic and to a lesser extent the likelihood root start to appear when $\sigma^2 \geq 10^{-1}$, with the left-tail error systematically too high and the right-tail error systematically too low. The modified root behaves much better overall, though it too loses accuracy in the right tail for larger values of $\sigma^2$. This is less consequential than error in the opposite tail, since tests of $H_0$ require accuracy on the left tail.

These remarks are confirmed by the Gaussian QQ-plots of simulated values of the three quantities in Fig 3. Poor lower-tail performance of a pivot will translate into poor error rates at the upper tail of the confidence interval, as we see from the reversal of limits in computing $I_{1-2\alpha}$ in Section III.A. If the distribution is exactly Gaussian, then the confidence intervals are exactly calibrated, so a departure from the line of unit slope through the origin implies a lack of calibration. Again we see that for small values of $\sigma^2$, all three statistics have standard normal distributions and give comparable results. For larger $\sigma^2$, the Wald statistic and the likelihood root are shifted to the right and right-skewed, more strikingly for larger values of $\tau$. This explains the asymmetric error rates in Table 4 with lower probabilities for the right than for the left. The asymmetry increases with larger uncertainties on the relative distance and velocity and with smaller nominal error rates.
The third column of Fig. 3 shows that the modified likelihood root $r^*$ corrects the departure from normality in the upper tail even for $\sigma^2 = 5$, and its error rates are closer to the nominal rates for all values considered. For $\sigma^2 > 2$ and for 1% nominal levels, the Wald statistic and the likelihood root show extreme overcoverage on the right and undercoverage on the left; although the modified likelihood root provides a considerable improvement its right non-coverage is somewhat smaller than the nominal value.

C. Scenario 2

Our second scenario is based on Table 2. Table 5 gives left and right error rates for different values of $\sigma^2$ and $\tau$. Its first row corresponds to the case where the standard deviation of the position error along each axis is 10 m and the standard deviation of the velocity errors is 10 m/s, giving $(\sigma, \tau) = (10^{-2}, 1)$. In subsequent rows we first increase uncertainty on the position while keeping uncertainty on the velocity fixed by increasing $\tau$, and then increase both velocity and position errors by increasing $\sigma^2$. For the specific geometry of this example we take a true miss distance of $\psi = 698$ m and relative velocity with norm $||v|| = 11.648 \times 10^3$ m/s, so the errors we consider vary from 10 to 200 for both velocity (m/s) and distance (m). The case where $(\sigma^2, \tau) = (10^{-4}, 10^2)$ is considered in Chen et al. [11, Chapter 2] as an initial orbital error. The authors assume that the error covariance matrix at any time can be obtained as quadratic propagation of the initial matrix through a transition function of time.

Table 5 shows that the error rates for the Wald statistic and the likelihood root are almost identical, implying that the corresponding pivots are indistinguishable. For small velocity errors, with $\sigma^2 < 10^{-3}$, there is no significant difference in the error rates for the three statistics. For larger velocity variance, although the overall error rates found by summing the left and the right error rates equal the nominal values, left error always dominates the sum. In these cases the modified likelihood root is more symmetric and shows fewer extreme values, especially for large $\tau$. Interval estimates based on $r^*$ are more reliable.

Point estimates of the miss distance and the probability of collision and one-sided $(1 - \alpha)$ confidence intervals of the forms $[L_\alpha, +\infty)$ or $[0, U_\alpha)$ lose information about the accuracy of the estimate, relative to two-sided intervals $[L_\alpha, U_\alpha]$. Such intervals convey more information about the quality of the estimates, giving operators more informative quantities for risk assessment and decision-making.
Table 4  Left and right error rates (%) for two-sided nominal 10%, 5%, and 1% confidence intervals for the true parameter $\psi_0$, estimated from $10^4$ Monte Carlo samples.

| Uncertainty | Statistic | Left tail (%) | Right tail (%) |
|-------------|-----------|---------------|----------------|
|             |           | 5  | 2.5 | 0.5 | 5  | 2.5 | 0.5 |
| $(\sigma^2, \tau) = (10^{-3}, 1)$ | Wald | 5.22 | 2.58 | 0.54 | 5.03 | 2.49 | 0.49 |
| | $r$ | 5.20 | 2.56 | 0.53 | 5.04 | 2.51 | 0.50 |
| | $r^*$ | 5.15 | 2.54 | 0.53 | 5.13 | 2.54 | 0.51 |
| $(\sigma^2, \tau) = (10^{-3}, 2)$ | Wald | 5.43 | 2.61 | 0.43 | 4.96 | 2.61 | 0.59 |
| | $r$ | 5.43 | 2.61 | 0.43 | 4.98 | 2.61 | 0.61 |
| | $r^*$ | 5.40 | 2.58 | 0.43 | 5.02 | 2.62 | 0.62 |
| $(\sigma^2, \tau) = (10^{-3}, 3)$ | Wald | 4.93 | 2.48 | 0.53 | 4.83 | 2.46 | 0.54 |
| | $r$ | 4.91 | 2.47 | 0.52 | 4.88 | 2.46 | 0.55 |
| | $r^*$ | 4.85 | 2.40 | 0.50 | 4.90 | 2.49 | 0.55 |
| $(\sigma^2, \tau) = (10^{-1}, 1)$ | Wald | 5.45 | 2.88 | 0.64 | 4.15 | 2.09 | 0.37 |
| | $r$ | 5.26 | 2.78 | 0.59 | 4.27 | 2.15 | 0.37 |
| | $r^*$ | 4.89 | 2.53 | 0.54 | 4.65 | 2.37 | 0.42 |
| $(\sigma^2, \tau) = (10^{-1}, 2)$ | Wald | 5.62 | 2.98 | 0.67 | 4.60 | 2.28 | 0.50 |
| | $r$ | 5.48 | 2.75 | 0.61 | 4.70 | 2.32 | 0.54 |
| | $r^*$ | 5.06 | 2.48 | 0.54 | 5.06 | 2.56 | 0.64 |
| $(\sigma^2, \tau) = (10^{-1}, 3)$ | Wald | 5.66 | 2.86 | 0.65 | 4.49 | 2.26 | 0.49 |
| | $r$ | 5.54 | 2.70 | 0.63 | 4.58 | 2.35 | 0.50 |
| | $r^*$ | 5.06 | 2.50 | 0.59 | 4.92 | 2.57 | 0.53 |
| $(\sigma^2, \tau) = (1, 1)$ | Wald | 7.21 | 4.10 | 1.04 | 3.18 | 1.37 | 0.16 |
| | $r$ | 6.45 | 3.36 | 0.68 | 3.35 | 1.53 | 0.21 |
| | $r^*$ | 5.39 | 2.64 | 0.55 | 4.56 | 2.37 | 0.31 |
| $(\sigma^2, \tau) = (1, 2)$ | Wald | 6.58 | 3.72 | 0.92 | 3.64 | 1.50 | 0.24 |
| | $r$ | 5.92 | 3.16 | 0.57 | 3.80 | 1.62 | 0.29 |
| | $r^*$ | 4.81 | 2.40 | 0.41 | 5.32 | 2.59 | 0.48 |
| $(\sigma^2, \tau) = (1, 3)$ | Wald | 6.40 | 3.50 | 0.96 | 3.73 | 1.64 | 0.25 |
| | $r$ | 5.74 | 3.03 | 0.64 | 3.94 | 1.76 | 0.25 |
| | $r^*$ | 4.74 | 2.49 | 0.54 | 5.19 | 2.72 | 0.46 |
| $(\sigma^2, \tau) = (2, 1)$ | Wald | 7.78 | 4.57 | 1.41 | 2.12 | 0.69 | 0.03 |
| | $r$ | 6.52 | 3.56 | 0.78 | 2.27 | 0.75 | 0.03 |
| | $r^*$ | 5.19 | 2.64 | 0.58 | 4.46 | 1.85 | 0.10 |
| $(\sigma^2, \tau) = (2, 2)$ | Wald | 7.94 | 4.59 | 1.33 | 2.30 | 0.71 | 0.05 |
| | $r$ | 6.77 | 3.49 | 0.71 | 2.43 | 0.88 | 0.05 |
| | $r^*$ | 5.18 | 2.60 | 0.54 | 4.62 | 2.09 | 0.18 |
| $(\sigma^2, \tau) = (2, 3)$ | Wald | 7.67 | 4.07 | 1.15 | 2.19 | 0.73 | 0 |
| | $r$ | 6.49 | 3.24 | 0.65 | 2.39 | 0.86 | 0 |
| | $r^*$ | 4.71 | 2.34 | 0.49 | 4.48 | 1.98 | 0.11 |
| Standard error | 0.22 | 0.16 | 0.07 | 0.22 | 0.16 | 0.07 |
Fig. 3  Gaussian QQ-plots of the Wald statistic (left column), the likelihood root (middle column) and modified likelihood root (right column) based on $10^4$ Monte Carlo sample quantiles. Top row ($\sigma^2, \tau = (10^{-3}, 1)$; second row ($\sigma^2, \tau = (1, 1)$; third row ($\sigma^2, \tau = (5, 2)$; bottom row ($\sigma^2, \tau = (5, 5)$).
Table 5  Left and right error rates (%) for two-sided nominal 10%, 5%, and 1% confidence intervals for the parameter \( \psi \) of the U.S. and Russian satellites collision event, based on 10^4 Monte Carlo replications.

| Uncertainty     | Statistic | Left tail (%) | Right tail (%) |
|-----------------|-----------|---------------|----------------|
| \((\sigma^2, \tau) = (10^{-4}, 1)\) | Wald      | 5.06 2.54 0.42 | 5.00 2.53 0.64 |
|                 | \(r\)     | 5.06 2.54 0.42 | 5.00 2.53 0.64 |
|                 | \(r^*\)   | 4.98 2.46 0.41 | 5.05 2.62 0.65 |
| \((\sigma^2, \tau) = (10^{-4}, 2)\) | Wald      | 5.27 2.73 0.60 | 4.66 2.29 0.52 |
|                 | \(r\)     | 5.27 2.73 0.60 | 4.66 2.290 0.52 |
|                 | \(r^*\)   | 5.17 2.67 0.56 | 4.78 2.33 0.53 |
| \((\sigma^2, \tau) = (10^{-4}, 4)\) | Wald      | 4.67 2.29 0.49 | 4.53 2.34 0.43 |
|                 | \(r\)     | 4.67 2.29 0.49 | 4.53 2.34 0.43 |
|                 | \(r^*\)   | 4.58 2.21 0.47 | 4.67 2.40 0.47 |
| \((\sigma^2, \tau) = (10^{-4}, 10^2)\) | Wald      | 5.89 2.98 0.74 | 4.33 2.05 0.47 |
|                 | \(r\)     | 5.89 2.98 0.74 | 4.33 2.05 0.47 |
|                 | \(r^*\)   | 5.18 2.73 0.65 | 5.14 2.59 0.61 |
| \((\sigma^2, \tau) = (10^{-3}, 1)\) | Wald      | 5.17 2.66 0.50 | 4.60 2.16 0.40 |
|                 | \(r\)     | 5.17 2.66 0.50 | 4.60 2.16 0.40 |
|                 | \(r^*\)   | 4.96 2.55 0.45 | 4.88 2.37 0.44 |
| \((\sigma^2, \tau) = (10^{-3}, 2)\) | Wald      | 5.00 2.50 0.48 | 4.93 2.35 0.37 |
|                 | \(r\)     | 5.00 2.50 0.48 | 4.93 2.35 0.37 |
|                 | \(r^*\)   | 4.76 2.34 0.45 | 5.31 2.54 0.42 |
| \((\sigma^2, \tau) = (10^{-3}, 4)\) | Wald      | 5.25 2.73 0.61 | 4.54 2.23 0.38 |
|                 | \(r\)     | 5.25 2.73 0.61 | 4.54 2.23 0.38 |
|                 | \(r^*\)   | 4.74 2.52 0.52 | 5.00 2.45 0.43 |
| \((\sigma^2, \tau) = (10^{-2}, 1)\) | Wald      | 5.75 2.96 0.54 | 4.53 2.06 0.31 |
|                 | \(r\)     | 5.75 2.96 0.54 | 4.54 2.07 0.32 |
|                 | \(r^*\)   | 5.09 2.56 0.44 | 5.33 2.70 0.43 |
| \((\sigma^2, \tau) = (10^{-2}, 2)\) | Wald      | 5.96 2.94 0.51 | 3.69 1.92 0.30 |
|                 | \(r\)     | 5.96 2.94 0.51 | 3.69 1.92 0.30 |
|                 | \(r^*\)   | 4.89 2.39 0.38 | 4.87 2.53 0.49 |
| \((\sigma^2, \tau) = (10^{-2}, 4)\) | Wald      | 6.20 3.26 0.57 | 2.73 1.14 0.0 |
|                 | \(r\)     | 6.20 3.26 0.57 | 2.73 1.14 0.0 |
|                 | \(r^*\)   | 4.78 2.45 0.41 | 4.96 2.30 0.31 |
| Standard error  |           | 0.22 0.16 0.07 | 0.22 0.16 0.07 |
VI. Further remarks

A. Summary

In this paper we formulated the relative motion problem in statistical terms, discussed approximate likelihood inference on the miss distance, and studied the repeated-sampling properties of confidence sets of special importance in conjunction assessment. Using two examples, we showed that standard likelihood-based confidence intervals can be quite poor, especially when uncertainty on the relative distance and velocity is large, but an improved approximation gives appreciably better inferences by compensating for the skewed distributions. We propose that the estimated conjunction probability be replaced by a significance probability for testing that the true miss distance is larger than a specified safety threshold; this significance probability is calibrated in a well-defined sense and provides a statistically well-founded basis for avoidance decisions.

Below we discuss some possible extensions of our ideas.

B. Successive observations

In practice successive six-dimensional observation vectors \( y_1, \ldots, y_n \) and corresponding \( 6 \times 6 \) variance matrices \( \Omega_1^{-1}, \ldots, \Omega_n^{-1} \) are typically available, with the variance matrices increasingly concentrated as information accrues on a conjunction. If the observations can be regarded as independent, then the corresponding log likelihood is

\[
\ell(\psi, \lambda_1, \ldots, \lambda_n) = -\frac{1}{2} \sum_{j=1}^{n} \{ y_j - \eta(\theta_j) \}^T \Omega_j \{ y_j - \eta(\theta_j) \},
\]

where \( \theta_j = (\psi, \lambda_j) \), with \( \psi \) representing the miss distance common to all the observations and \( \lambda_1, \ldots, \lambda_n \) representing the \( n \times 1 \) vectors of nuisance parameters corresponding to \( y_1, \ldots, y_n \). The more precise \( y_j \) are automatically given higher weight, since the corresponding dispersion matrices \( \Omega_j \) are larger. In this case the overall parameter vector is \( \theta = (\psi, \lambda_1, \ldots, \lambda_n) \), and the approach of Section IV can be applied with minor changes.

More complicated geometry leading to a different form for \( \eta(\theta_j) \) would be needed if the relative motions for the observations could not be considered to be rectilinear.

C. Decision analysis

Conjunction assessment is used to inform decisions on satellite manoeuvres to avoid collisions, and this can be formalised in a simple decision framework, with two possible actions \( a = 0 \) and \( a = 1 \) corresponding to ‘do nothing’ and ‘take evasive action’ and with loss function \( l_{ae} \) for the loss when action \( a \) is taken and event \( e \) occurs given in Table 6; we suppose that the loss in doing nothing in the case of no collision is zero. In a Bayesian framework and supposing that
Table 6  Basic decision analysis for satellite conjunction, with losses $l_{ae}$ corresponding to action $a$ and event $e$.

| Action          | Event     | No collision | Collision |
|-----------------|-----------|--------------|-----------|
| Do nothing, $a=0$ | $l_{00}=0$ | $l_{01}$     |           |
| Evasive action, $a=1$ | $l_{10}$  | $l_{11}$     |           |

$\psi \leq \psi_0$ results in a collision, the posterior loss for action $a$ is

$$l_{a0}\Pr(\psi > \psi_0 \mid y) + l_{a1}\Pr(\psi \leq \psi_0 \mid y) = l_{a0}(1-p) + l_{a1}p,$$

say, which is to be minimised over $a$. The posterior loss is minimised by doing nothing, action $a=0$, if $pl_{01} < (1-p)l_{10} + pl_{11}$ and otherwise by evasive action, $a=1$. As the significance probability $p_{obs}$ provides a close approximation to $p$, the posterior loss is therefore approximately minimised by taking evasive action if $p_{obs} \geq l_{10}/(l_{10} + l_{01} - l_{11})$.

D. Conjunction geometry

It may appear puzzling that although the calculation of the estimated collision probability $\widehat{p}_c$ involves integration over an ellipse, no such computation is needed above. However, the conjunction geometry implicitly plays a role in the calculation of $p_{obs}$, which depends on the covariance matrix of the conjunction. A more detailed geometric discussion going beyond using the combined hard body radius is possible in principle, but would require data on the relative angular velocity of the two space objects.

Appendix A: Theoretical background

The key to improving first-order approximations is to account for the presence of nuisance parameters. One important improvement, the modified likelihood root [27, 28], is given by equation (10). If the response distribution is continuous and has true parameter $\psi_0$, then $r^*(\psi_0)$ is asymptotically standard normal to order $O(n^{-3/2})$. If we follow Barndorff-Nielsen and Cox [27, chapter 5] and assume that there is a map from the data $y$ to $(\widehat{\theta}, a)$, where $a$ is a complementary statistic which is either exactly or approximately ancillary, then the log-likelihood function can be written as $\ell(\theta; y) = \ell(\theta; \widehat{\theta}, a)$ and the correction term needed in (10) may be expressed as

$$q(\psi) = \left| \ell_{,\widehat{\theta}}(\overline{\widehat{\theta}}) - \ell_{,\overline{\widehat{\theta}}} \left( \overline{\widehat{\theta}} \right) \ell_{,\overline{\overline{\widehat{\theta}}}} \left( \overline{\widehat{\theta}} \right) \right| / \left| J(\overline{\widehat{\theta}}) \right|^{1/2},$$

where $\ell_{,\widehat{\theta}}(\theta) = \partial \ell(\theta; \widehat{\theta}, a)/\partial \widehat{\theta}$ is a sample space derivative and quantities such as $\ell_{,\overline{\widehat{\theta}}}(\theta) = \partial^2 \ell(\theta; \widehat{\theta}, a)/\partial \theta \partial \overline{\widehat{\theta}}$ are referred to as mixed derivatives. For more detailed discussion see Barndorff-Nielsen and Cox [27, Chapters 5 and 6].

The difficulty with (19) is that a transformation from $y$ to $(\widehat{\theta}, a)$ may be unavailable. If so, then the tangent
exponential model proposed by Fraser and co-authors [e.g., 28] may be used. This is based on a local exponential family approximation to the log-likelihood function for $n$ independent observations $y_1, \ldots, y_n$ that has $d \times 1$ canonical parameter

$$
\varphi^T(\theta) = \ell_V(\theta; y^o) = V^T \sum_{i=1}^{n} \frac{\partial \ell(\theta; y_i)}{\partial y_i} y_i V_i,
$$

(20)

and involves a directional derivative of the log-likelihood function evaluated at the observed data point $y^o = (y_1^o, \ldots, y_n^o)^T$, as $\ell_V(\theta; y^o)$ is the derivative of $\ell(\theta)$ in the directions given by the $n$ rows $V_1, \ldots, V_n$ of the $n \times d$ matrix $V$. This matrix can be constructed using a vector of pivotal quantities $z \equiv z(y; \theta) = \{z_1(y_1, \theta), \ldots, z_n(y_n, \theta)\}^T$ through

$$
V = \frac{\partial y}{\partial \theta^T} \bigg|_{y=y^o, \theta=\theta^o} = - \left( \frac{\partial z}{\partial y^T} \right)^{-1} \bigg|_{y=y^o, \theta=\theta^o} \times \frac{\partial z}{\partial \theta^T} \bigg|_{y=y^o, \theta=\theta^o},
$$

(21)

where $\theta^o$ is the maximum likelihood estimate at $y^o$. The tangent exponential model implicitly depends on the approximate ancillary statistic $a$ which varies locally at its observed value $a^o$ in the $n - d$ directions orthogonal to the columns of $V$. The resulting correction term can be written in the form [13]. The numerator of the first term of $q$ is the determinant of a $d \times d$ matrix whose first column is $\varphi(\hat{\theta}) - \varphi(\hat{\theta}_\psi)$ and whose remaining columns are $\varphi_1(\hat{\theta}_\psi)$. Further details can be found in Brazzale et al. [12, Section 8.5] and a guide to the literature may be found in Davison and Reid [29].

### Appendix B: Cartesian coordinates

In reparametrizing the model to $(\psi, \lambda)$, it is important to ensure that the parameter space $\theta$ for $\theta$ is preserved by the transformation. In particular, when $\theta = \Psi \times \Lambda$, where $\Psi$ and $\Lambda$ are the parameter spaces for $\psi$ and $\lambda$, we say that the parametrization is variation independent. If the allowable values of $\psi$ were to depend on $\lambda$, this would introduce irregularities into the model and the usual asymptotic theory would not apply. We show below that this is the case when the miss distance $\psi$ is expressed in Cartesian coordinates.

Assume that the relative position and relative velocity vectors given in the Cartesian coordinate system are $(\mu, v) = (\mu_1, \mu_2, \mu_3, v_1, v_2, v_3)$. If we express one component, for example $\mu_1$, in terms of $\psi$ and the other parameters,
then we have

\[ \psi^2 = \mu^T \mu - \left( \mu^T v \right)^2 / v^T v, \]

\[ = \mu_1^2 + \mu_2^2 + \mu_3^2 - (\mu_1 v_1 + \mu_2 v_2 + \mu_3 v_3)^2 / (v_1^2 + v_2^2 + v_3^2), \]

\[ = \mu_1^2 \left( \frac{v_2^2 + v_3^2}{v_1^2 + v_2^2 + v_3^2} \right) + \mu_2^2 \left( \frac{v_1^2 + v_3^2}{v_1^2 + v_2^2 + v_3^2} \right) + \mu_3^2 \left( \frac{v_1^2 + v_2^2}{v_1^2 + v_2^2 + v_3^2} \right) - 2 \mu_1 \frac{v_1 (v_2 \mu_2 + v_3 \mu_3)}{v_1^2 + v_2^2 + v_3^2} - 2 \mu_2 v_2 \mu_3 v_3 \frac{\nu}{v_1^2 + v_2^2 + v_3^2}, \]

\[ = A \mu_1^2 - 2B \mu_1 + C, \]

where

\[ A = \frac{v_2^2 + v_3^2}{v_1^2 + v_2^2 + v_3^2}, \quad B = \frac{v_1 (v_2 \mu_2 + v_3 \mu_3)}{v_1^2 + v_2^2 + v_3^2}, \quad C = \frac{v_1^2 (\mu_2^2 + \mu_3^2) + (\mu_2 v_3 - \mu_3 v_2)^2}{v_1^2 + v_2^2 + v_3^2}. \]

This implies that \( \mu_1 \) solves the quadratic equation \( A \mu_1^2 + 2B \mu_1 + (C - \psi^2) = 0 \), i.e.,

\[ \mu_1 = \frac{B \pm \sqrt{D}}{A}, \quad D = B^2 + A(\psi^2 - C), \]

which can be simplified to

\[ \mu_1 = \frac{v_1 (v_2 \mu_2 + v_3 \mu_3) \pm \sqrt{\Delta}}{v_2^2 + v_3^2}, \]

where

\[ \Delta = v_1^2 (v_2 \mu_2 + v_3 \mu_3)^2 + \left[ \psi^2 (v_1^2 + v_2^2 + v_3^2) - \{v_1^2 (\mu_2^2 + \mu_3^2) + (\mu_2 v_3 - \mu_3 v_2)^2\}\right] (v_2^2 + v_3^2) \]

\[ = v^T \{ \psi^2 (v_2^2 + v_3^2) - (\mu_2 v_3 - \mu_3 v_2)^2 \} \]

which will give an expression for \( \mu_1 \) in terms of the interest parameter \( \psi \) and the nuisance parameter \( \lambda = (\mu_2, \mu_3, v_1, v_2, v_3) \).

Note, however, that we require that \( \Delta > 0 \), which implies that we must have \( \psi^2 > (\mu_2 v_3 - \mu_3 v_2)^2 / (v_2^2 + v_3^2) \), and this is only zero if \( (\mu_2, \mu_3) \) and \( (v_2, v_3) \) are colinear, in which case the satellite can pass through the origin. To see this another way, \( (\mu_2 v_3 - \mu_3 v_2) / (v_2^2 + v_3^2)^{1/2} \) is the projection of \( (\mu_2, \mu_3) \) onto a unit vector \( (-v_3, v_2) / (v_2^2 + v_3^2)^{1/2} \) orthogonal to \( (v_2, v_3) \).

The above expressions give two possible values for \( \mu_1 \), but the geometry implies that we must choose the solution for which \( \mu^T v < 0 \), as otherwise the satellite is heading away from the origin. For any specified distance \( \psi \) greater than the shortest distance, for which \( \Delta = 0 \), it is clear from the geometry that if \( v_1 > 0 \) then we should take the root with the
written in the form which implies that the root for which the argument is that if \( \nu_1 > 0 \) and we denote the two roots by \( \mu_1^+ \) and \( \mu_1^- = \mu_1^+ + 2\Delta', \) where \( \Delta' > 0, \) then

\[
\mu_1^+ \nu_1 + \mu_2 \nu_2 + \mu_3 \nu_3 = \mu_1^- \nu_1 + \mu_2 \nu_2 + \mu_3 \nu_3 + 2\nu_1 \Delta' > \mu_1^- \nu_1 + \mu_2 \nu_2 + \mu_3 \nu_3,
\]

which implies that the root for which \( \mu^+ \nu < 0 \) must be given by \( \mu_1^- \). Likewise, we should choose \( \mu_1^- \) if \( \nu_1 < 0. \)

The constraint on \( \psi \) implies that it is not variation independent of \( \lambda, \) in the sense that for \( \theta = (\psi, \lambda) \) we do not have \( \theta \in \Psi \times \Lambda \) where \( \theta, \Psi \) and \( \Lambda \) are the parameter sets for \( \theta, \psi \) and \( \lambda. \) This causes problems when eliminating \( \lambda \) from the log-likelihood function.

### Appendix C: Analytical details

In order to obtain the matrix \( V \) used in the tangent exponential model approximation we define the vector of pivots as \( z(y, \theta) = \Omega^{1/2} \{y - \eta(\theta)\}, \) which are independent and standard normal under the model. Partial differentiation yields

\[
V = \frac{\partial \eta(\theta)}{\partial \theta} = \eta_{\theta}(\theta),
\]

evaluated at the maximum likelihood estimate \( \hat{\theta}^0 \) corresponding to \( y^0. \) The log-likelihood, \(-\frac{1}{2}(y - \eta)^T \Omega(y - \eta),\) has derivative \( \Omega(\eta - y) \) with respect to \( y, \) so from \((20)\) the canonical parameter of the tangent exponential model may be written in the form \( \varphi(\hat{\theta}) = B\eta(\hat{\theta}) + a, \) where \( B = -\eta_{\theta}^T(\hat{\theta}^0)\Omega \) and \( a = \eta_{\theta}^T(\hat{\theta}^0)\Omega y^0 \) are both constant with respect to \( \theta \) and \( B \) is full-rank. Any canonical parameter that is an affine transformation of \( \eta \) gives the same expression for \( q(\psi), \)

\[
\left| \begin{array}{c} \varphi(\hat{\theta}) - \varphi(\tilde{\theta}_\psi) \\ \varphi_{\theta}(\tilde{\theta}) \\ \varphi_{\theta}(\tilde{\theta}) \end{array} \right| = B \left| \begin{array}{c} \eta(\hat{\theta}) - \eta(\tilde{\theta}_\psi) \\ \eta_{\theta}(\tilde{\theta}) \\ \eta_{\theta}(\tilde{\theta}) \end{array} \right| B_{\eta_{\theta}}(\tilde{\theta}) = \left| \begin{array}{c} \eta(\hat{\theta}) - \eta(\tilde{\theta}_\psi) \\ \eta_{\theta}(\tilde{\theta}) \\ \eta_{\theta}(\tilde{\theta}) \end{array} \right| B_{\eta_{\theta}}(\tilde{\theta}),
\]

where \( \eta_{\theta}(\hat{\theta}) = \frac{\partial \eta(\hat{\theta})}{\partial \theta}. \) Hence we can take the constructed parameter to be \( \varphi(\hat{\theta}) = \eta(\hat{\theta}). \) To compute \((22)\), we need the \( 6 \times 6 \) Jacobian \( \eta_{\theta} \) and the second derivatives \( \eta_{\theta \theta}, \) a \( 6 \times 6 \times 6 \) tensor containing the second derivatives of \( \eta, \) which is needed to compute \( j_{\lambda_1}(\hat{\theta}_\psi). \) The score equation and the observed Fisher information can respectively be given as

\[
\frac{\partial \eta_{\theta}(\theta)}{\partial \theta} \Omega(y - \eta(\theta)) = 0, \quad \frac{\partial^2 \eta_{\theta}(\theta)}{\partial \theta^2} \Omega(y - \eta(\theta)) - \frac{\partial^2 \eta_{\theta}(\theta)}{\partial \theta \partial \theta} \Omega(y - \eta(\theta)), \quad r = 1, \ldots, 6.
\]
The expected information matrix, the expectation of the observed information matrix, equals $\eta^T(\theta)\Omega\eta(\theta)$ because $E(y) = \eta(\theta)$. The observed information matrix evaluated at the maximum likelihood estimate for the full model equals $j(\hat{\theta}) = \eta^T(\hat{\theta})\Omega\eta(\hat{\theta})$, because the score equation for the full model implies that $\eta(\hat{\theta}) = y$.

A fuller version of a similar computation is in Fraser et al. [30].

**Appendix D: Bayesian approximation**

The derivation of equation (17) is outlined in Section 8.7 of Brazzale et al. [12]. As $\hat{\theta}^\top = (\psi, \tilde{\lambda}_\psi)$,

$$
\frac{dl(\hat{\theta}_\psi)}{d\psi} = \ell_\psi(\hat{\theta}_\psi) + \frac{\partial^2\ell_\psi}{\partial\psi}\ell_\lambda(\hat{\theta}_\psi) = \ell_\psi(\hat{\theta}_\psi) - \ell_{\psi,\lambda}(\hat{\theta}_\psi)\ell^{-1}_{\lambda,\lambda}(\hat{\theta}_\psi)\ell_{\lambda}(\hat{\theta}_\psi),
$$

where subscripts on $\ell$ denote partial differentiation and the second equality follows from noting that differentiating the equation $\ell_\lambda(\hat{\theta}_\psi) = 0$ that defines $\tilde{\lambda}_\psi$ yields

$$
\ell_{\psi,\lambda}(\hat{\theta}_\psi) + \frac{\partial^2\ell_\psi}{\partial\psi}\ell_{\lambda,\lambda}(\hat{\theta}_\psi) = 0,
$$

with the matrix $\ell_{\lambda,\lambda}(\hat{\theta}_\psi)$ invertible because it is the Hessian corresponding to the maximum of $\ell$ in the $\lambda$ direction for fixed $\psi$. A standard identity for the determinant of a partitioned matrix gives

$$
\begin{bmatrix}
\ell_\theta(\hat{\theta}_\psi) & \ell_{\theta,\lambda}(\hat{\theta}_\psi) \\
\ell_{\lambda}(\hat{\theta}_\psi) & \ell_{\lambda,\lambda}(\hat{\theta}_\psi)
\end{bmatrix}
= \begin{bmatrix}
\ell_\theta(\hat{\theta}_\psi) & \ell_{\theta,\lambda}(\hat{\theta}_\psi) \\
\ell_{\lambda}(\hat{\theta}_\psi) & \ell_{\lambda,\lambda}(\hat{\theta}_\psi)
\end{bmatrix}
\begin{bmatrix}
\ell_\theta(\hat{\theta}_\psi) - \ell_{\theta,\lambda}(\hat{\theta}_\psi)\ell^{-1}_{\lambda,\lambda}(\hat{\theta}_\psi)\ell_{\lambda}(\hat{\theta}_\psi)
\end{bmatrix}
\begin{bmatrix}
\ell_{\lambda,\lambda}(\hat{\theta}_\psi)
\end{bmatrix}, \quad (24)
$$

and the expression for the observed information in (23) implies that we can write

$$
-\ell_{\theta,\lambda}(\hat{\theta}) = \eta^T(\hat{\theta})\Omega\eta_{\lambda,\lambda}(\hat{\theta}) + A_r(\hat{\theta})\{y - \eta(\hat{\theta})\}, \quad r = 1, \ldots, d - 1,
$$

where $A(\hat{\theta})$ involves second derivatives of $\eta$. Now $y = \eta(\hat{\theta})$, so if $\hat{\psi} - \psi$ is of order $n^{-1/2}$, then $y - \eta(\hat{\theta}) = \eta(\hat{\theta}) - \eta(\hat{\theta})$ is also $O(n^{-1/2})$, and hence so too is the second term of $-\ell_{\theta,\lambda}(\hat{\theta})$. Thus (24) equals

$$
\begin{bmatrix}
\ell_\theta(\hat{\theta}_\psi) & \ell_{\theta,\lambda}(\hat{\theta}_\psi)
\end{bmatrix}
= (-1)^{d-1}\begin{bmatrix}
\ell_\theta(\hat{\theta}_\psi) & -\ell_{\theta,\lambda}(\hat{\theta}_\psi)
\end{bmatrix}
$$

$$
= (-1)^{d-1}\begin{bmatrix}
\eta_\theta(\hat{\theta}_\psi)\Omega_{y - \eta(\hat{\theta}_\psi)} & \eta^T_\theta(\hat{\theta}_\psi)\Omega_{\eta_{\lambda,\lambda}(\hat{\theta}_\psi)} + O(n^{-1/2}),
\end{bmatrix}
$$

$$
= (-1)^{d-1}\begin{bmatrix}
\eta_\theta(\hat{\theta}_\psi) & [\Omega]_{\eta(\hat{\theta}) - \eta(\hat{\theta}_\psi)} + O(n^{-1/2})
\end{bmatrix}
\begin{bmatrix}
\eta_\lambda(\hat{\theta}_\psi)
\end{bmatrix}.
$$

23
As \( \theta \) is of dimension \( d \) and \( |J(\tilde{\theta})| = \left| \eta_\theta^T(\tilde{\theta}) \right|^2 \left| \Omega \right| \), equation (17) equals

\[
q_B(\psi) = \frac{|\ell_\theta(\tilde{\theta}_\psi) - \ell_{\theta,1}(\tilde{\theta}_\psi)|}{|J_{\theta,1}(\tilde{\theta}_\psi)|^{1/2} |J(\tilde{\theta})|^{1/2}} \times \frac{\pi(\tilde{\theta})}{\pi(\tilde{\theta}_\psi)},
\]

\[
= \frac{|\eta_\theta(\tilde{\theta}_\psi)| |\Omega| \left| \eta(\tilde{\theta}) - \eta(\tilde{\theta}_\psi) \right|}{|J_{\theta,1}(\tilde{\theta}_\psi)|^{1/2} |J(\tilde{\theta})|^{1/2} \left| \eta_\theta^T(\tilde{\theta}) \right|^{1/2}} \times \frac{\pi(\tilde{\theta})}{\pi(\tilde{\theta}_\psi)} + O(n^{-1/2}),
\]

\[
= q(\psi) \times \frac{|\eta_\theta^T(\tilde{\theta}_\psi)|}{|\eta_\theta^T(\tilde{\theta})|} \times \frac{\pi(\tilde{\theta})}{\pi(\tilde{\theta}_\psi)} + O(n^{-1/2}).
\]

where \( q(\psi) \) is given in equation (13).

The Jeffreys prior is the root of the determinant of the Fisher information matrix,

\[
\pi(\theta) \propto |\eta^T_\theta(\theta) \Omega \eta_\theta(\theta)|^{1/2} \propto |\eta_\theta(\theta)|,
\]

as the constant \( |\Omega| \) can be ignored. If this prior is used then (25) simplifies to equation (18), plus a term of \( O(n^{-1/2}) \).

Hence \( r_B(\psi) = r^*(\psi) + O(n^{-1}), \) and inferences from (14) and (16) will be the same to this order of error.

**Appendix E: Implementation details**

The main steps for the numerical implementation of higher-order quantities are:

1) Calculation of the log-likelihood \( \ell(\psi, \lambda) \) with \( \psi \) given in (3).
2) Computation of \( r_\psi(\psi), q^0(\psi) \) and \( r^{*0}(\psi) \) for a range of values of \( \psi \) around the maximum likelihood estimate \( \tilde{\psi}^0 \): at each point of the grid we perform a constrained optimization to obtain \( \tilde{\lambda}_\psi^0 \), which is then used in (22) to evaluate the pivots.
3) Interpolation of the points by a smoothing method.
4) If desired, a point estimate \( \tilde{\psi}^{*0} \) of \( \psi \) can be obtained by solving the equation \( r^{*0}(\psi) = 0 \). This estimate is an improvement on the maximum likelihood estimate itself.
5) Inversion of the interpolating function to find the limits \( \psi_\alpha \) and \( \psi_{1-\alpha} \) of the \( 1 - 2\alpha \) confidence interval for \( \psi \).

For the constrained optimization, we use the ‘Rvmmin’ solver in optimr() function of the R package optimr. The algorithm is overall robust, fast, and less sensitive to perturbations in initial values compared to other solvers. Partial derivatives needed to compute (13) are obtained using Mathematica.
Very large values of $r^*$ that arose for around 1% of the simulated datasets due to numerical instabilities when $|r| < 0.05$ are excluded from the computations. Such tiny values of $r$ suggest that $\tilde{\psi} \approx \psi$, leading to significance levels of around 0.5, which are not of interest.

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