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A CONTINUOUS MULTIPLE HYPOTHESIS TESTING FRAMEWORK FOR OPTIMAL EXOPLANET DETECTION

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When searching for exoplanets, one wants to count how many planets orbit a given star, and determine what their orbital parameters are. If the estimated orbital elements are too far from those of a planet truly present, this should be considered as a false detection. This setting is a particular instance of a general one: aiming to retrieve which parametric patterns are in a dataset corrupted by nuisance signals, with a certain accuracy on their parameters. We search for a detection criterion minimizing false and missed detections, either as a function of their relative cost, or when the expected number of false detections is bounded. We find that if the patterns can be separated in a technical sense, it is sufficient to select the parameter regions with highest posterior probability. We then discuss how the obtained posterior probabilities can be calibrated. We apply our procedure to the retrieval of periodic signals in unevenly sampled time series, emulating the search for exoplanets in radial velocity data. We show on a simulation that, for a given tolerance to false detections, the new criterion leads to 15 to 30% more true detections than other criteria, including the Bayes factor.

1. Introduction. Planets outside the Solar System, or exoplanets, can be detected by several observational techniques, leading to different types of data (Perryman, 2018). In all cases, based on these data, the goal is to determine how many planets can be confidently detected and what their characteristics are: orbital period, eccentricity, mass, radius, etc. Even if the number of planets detected matches the true number of planets, if the orbital elements of a planet whose detection is claimed are too far from those of a planet truly in the system, it might lead to incorrect scientific conclusions. We thus need to tie the detection criterion to the desired accuracy on the orbital elements.

In the present work, we adopt a general parametric model encompassing exoplanets. The data is described by n=0 to n_{\max} signals, which we call patterns. The pattern i=1,...,n is described by the parameter vector θ_i . We further assume that the data is corrupted by nuisance signals, deterministic or stochastic, parametrized by a vector η . In the case of exoplanets, θ_i is the vector of orbital elements of planet i, and η could include instrument offsets (intercepts), and hyperparameters of a Gaussian process modelling the noise. We further suppose we have a likelihood function and a prior distribution on our variables n, $(\theta_i)_{i=1...n}$, η . The patterns need not be parametrized in the same way. For instance, we could simultaneously search for planets and moons.

Our aim is to determine which patterns are present in a dataset, and can be seen as an extension of the discrete Bayesian false discovery rate problem of Müller et al. (2004); Muller, Parmigiani and Rice (2006). They consider a dataset that can potentially support n out of m discrete hypotheses H_i , indexed by i = 1..m. Their goal is to find n, and a subset S of n

indices such that the claim "the n hypotheses $H_i, i \in S$ are true" is optimal in a certain sense. In our work, hypotheses are of the form: "there are n patterns, one with parameters in Θ_1 ,..., one with parameters in Θ_n ", where Θ_i s are regions of the parameter space. The Θ_i s can then be thought of as continuous indices.

If among the $(\Theta_i)_{i=1..n}$ chosen, p of them do not contain the parameters of a pattern truly present, we count p false detections. We then consider two definitions of missed detections, made explicit in Section 2.1. To optimize the choice of $(\Theta_i)_{i=1..n}$, as in Müller et al. (2004), we adopt two approaches. First, we compute the maximum utility action, where the objective function performs a trade-off between false and missed detections. Second, we minimise the expected number of missed detections subject to a constraint on the expected number of false ones. We find that provided the Θ_i s cannot be too close to each other in some sense, the optimal detection procedure simply consists in taking the Θ_i , i = 1..n such that for each i, the posterior probabilities of having a pattern with parameters in Θ_i is greater than a certain threshold.

As a posterior probability, our significance metric is particularly meaningful if it is calibrated. That is, if among detections with posterior probability α , on average a fraction α of them is correct. In the terms of Box (1980), while finding an optimal decision pertains to the "estimation" problem: selecting a decision among a of alternatives, calibration pertains to "model criticism": determining whether this set of alternatives is reasonable. We define a general test for model criticism, which we apply in the case of exoplanets, where such tests are rarely performed.

We illustrate our results with an exoplanet detection method poised to play a crucial role in the coming decades, in particular in the search for life outside the Solar System (Crass et al., 2021), the radial velocity (RV) technique. For the sake of simplicity, we here consider that detecting planets with the RV technique consists in finding parametric periodic signals in an unevenly sampled time series. We refer the reader to Hara and Ford (2023) for a more in-depth presentation of RV analysis.

The number of planet detections supported by an RV time series is often decided on the basis of a Bayes factor comparing the n+1 vs. n planets hypotheses (e.g. Gregory, 2007; Tuomi and Kotiranta, 2009; Brewer and Donovan, 2015; Díaz et al., 2016; Faria et al., 2016). Alternatively, one can use periodograms (Baluev, 2008; Zechmeister and Kürster, 2009; Baluev, 2009; Baluev, 2013; Baluev, 2015; Delisle, Hara and Ségransan, 2020a), (Hara et al., 2017) or sparse recovery techniques (Hara et al., 2017), associated to a false alarm probability. These statistical significance metrics do not explicitly encode that for a detection to be deemed valid, the orbital elements of the planets have to be close to the true ones with a certain accuracy. Our original motivation was to define a detection criterion which expresses as closely as possible that an exoplanet has been detected (Hara et al., 2022a).

The present work is organised as follows. In Section 2, we present our formalism. The optimal criterion is searched as a maximum utility action in Section 3 and minimum missed detection under constraints on the number of false ones in Section 4. In Section 5, we present what the optimal procedure is, we show an example of application and discuss the relationship of our work with the Bayesian approaches to false discovery rates. We address the problem of model criticism and calibration in section 6, and conclude in Section 7.

2. Formalism. Let us consider a dataset $y \in \mathcal{Y}$, potentially exhibiting an unkown number of patterns n, such that pattern i = 1, ..., n is parametrized by vector $\theta_i \in T$. The parameters of the nuisance signals are denoted by $\eta \in H$. Our results are valid if \mathcal{Y} , T and H are measurable spaces, and in most practical cases their elements are real valued vectors.

To simplify notations, we denote by p(x) the distribution of the random variable x, instead of $p_X(x)$ for instance. We assume that we have a likelihood function $p(y \mid (\theta_i)_{i=1...n}, \eta)$ and

a proper prior distribution $p((\theta_i)_{i=1...n}, \eta)$. For a maximum of n_{max} patterns, the space onto which these distributions are defined is

(1)
$$\Theta = H \coprod H \times T \coprod H \times T^2 \coprod \dots \coprod H \times T^{n_{\text{max}}}$$

where \coprod represents the disjoint union. Here n_{\max} can be a positive integer or $+\infty$.

In the context of exoplanets, n is the number of planets and θ_i are the parameters of planet i. The parameters η is a vector including the instrumental offsets, potentially polynomial trends, hyperparameters of a stochastic process describing the noise, etc. The likelihood describes the noise model, and the priors are either reference ones, or aimed at representing the demographics of planets.

Supposing there are m different types of parameters, we can define $T=T^1 \coprod T^2 ... \coprod T^m$, the likelihood would then look like $p(\theta_i^1)_{i=1,...n_1},...,(\theta_i^m)_{i=1,...n_m},\eta\mid y)$ where $\theta_i^j\in T^j$. For instance, we might want to simultaneously search for planets, moons, comets around other stars.

2.1. *Detections*. To express that we want a certain accuracy on the pattern parameters, we define a detection claim as follows.

DEFINITION 2.1 (Detection claim). We first choose \mathcal{T} , a set of measurable subspaces of $T \coprod T^2 \coprod ... \coprod T^{n_{\max}}$. Given $(\Theta_1,...,\Theta_n) \in \mathcal{T}$, a detection claim is denoted by $a(\Theta_1,...,\Theta_n)$ and defined as the event "There are exactly n patterns, one with parameters in Θ_1 , one with parameters in Θ_2 ..., one with parameters in Θ_n ".

One of the possibilities, if T is a metric space, is to choose \mathcal{T} such that the Θ_i are closed balls of fixed radius. This conveys the idea that a certain resolution on the parameters is desired.

A detection claim is completely correct if there are n patterns truly present in the data, whose parameters $(\theta_i)_{i=1...n}$ are such that there exists a permutation of the indices σ with $\theta_{\sigma(i)} \in \Theta_i$ for all i=1,...,n. The permutation simply expresses that the order of the Θ_i s does not matter. The detection claim can also be partially incorrect. There can be false and missed detections, which we define as follows.

DEFINITION 2.2 (False detections). If for a detection claim of n patterns $(\Theta_i)_{i=1...n}$ for k of the Θ_i s which do not contain true parameters, we count k false detections.

We give two alternative definitions of missed detection. In the next sections, we discuss whether our results depend on a definition or the other.

DEFINITION 2.3 (Missed detections I). If n patterns are claimed, but in fact there are n' > n patterns truly present in the data, we count n' - n missed detections.

DEFINITION 2.4 (Missed detections II). If there are k signals truly in the data whose parameters are not contained in any of the Θ_i s, we count k missed detections.

2.2. The false inclusion probability. We will see that the choice of Θ_i s minimizing the number of errors involves the posterior probability of the event "there is one pattern with parameters in $\Theta_1 \subset T$ ", we denote this probability by I_{Θ_1} , and we have

(2)
$$I_{\Theta_1} := \sum_{k \ge 1} p(k \mid y) I_{\Theta_1}^k,$$

(3)
$$I_{\Theta_1}^k := \int_{\exists i, \theta_i \in \Theta_1} p(\theta_1, ..., \theta_k, \eta \mid y, k) \, \mathrm{d}\,\theta_1 ... \, \mathrm{d}\,\theta_k \, \mathrm{d}\,\eta$$

where $p(k \mid y)$ is the posterior probability of having k patterns. Some formulae are more conveniently written with the probability not to have a pattern in Θ_1 . Following Hara et al. (2022a) we call it the false inclusion probability (FIP), defined as

$$FIP_{\Theta_1} := 1 - I_{\Theta_1}.$$

The FIP can be seen as an extension of the posterior inclusion probability (PIP), applicable to linear models (Barbieri and Berger, 2004), to the general model considered here.

The quantity I_{Θ_1} in Eq. (2) is decomposed in terms $p(k \mid y)$ and $I_{\Theta_1}^k$ for $k = 0...n_{\text{max}}$. Those are easily computed as a by-product of the calculations necessary to evaluate the Bayesian evidence of the models with a fixed number k of patterns. Indeed, with notations of Eq. (2),

(5)
$$p(k \mid y) = \frac{p(y \mid k)p(k)}{\sum_{i=1}^{n_{\text{max}}} p(i \mid k)p(i)},$$

where p(i) is the prior probability to have i patterns, and

(6)
$$p(y|k) = \int p(y|k, \theta_1, ..., \theta_k, \eta) p(\theta_1, ..., \theta_k) d\theta_1 ... d\theta_k d\eta$$

is the Bayesian evidence, integrated on all possible combinations of k patterns. Furthermore, let us suppose that for a fixed k, there are N posterior samples of the distribution $p(\theta_1,...,\theta_k,\eta\mid y,k),\ \theta^i=(\theta_1^i,...,\theta_k^i),\ i=1...N,$ reliably exploring the parameter space. The quantity $I_{\Theta_1}^k$ in Eq. (3) can simply be estimated as the number of indexes i such that for some $j=1,...,k,\ \theta_j^i\in\Theta_1$, divided by the total number of samples N. Alternatively, $I_{\Theta_1}^k$ can be estimated with a nested sampler (Skilling, 2006). For a model with k patterns, nested samplers provide a collection of N samples $\theta^i=(\theta_1^i,...,\theta_k^i),\ i=1,...N$, associated to a weight w_i and a likelihood L_i . Denoting by $p_i=w_iL_i/\sum_j w_jL_j,\ I_{\Theta_1}^k$ in Eq. (3) is simply the sum of p_i taken over the indices of samples with θ^i such that $\theta_j^i\in\Theta_1$ for some j.

2.3. Example. To illustrate the notions given above, let us consider the radial velocity time-series of HD 21693 (Udry et al., 2019), taken with the HARPS instrument and processes with the YARARA pipeline (Cretignier et al., 2021). The RV technique consists in acquiring the spectrum of a given star at different times. Thanks to the Doppler effect, by measuring the frequency shift between these spectra astronomers can determine the variation of the radial velocity (RV) of the star: its velocity projected onto the line of sight. If an orbiting planet is present, it causes a reflex motion of its host star, and thus periodic RV variations. If several planets orbit the star, their combined effect is well approximated by the sum of their individual ones. Denoting by y the RV time series analysed, our likelihood is defined by the model of the measurement at time t,

(7)
$$y(t) = c_0 + \sum_{j=1}^{n} f(t, \theta_i) + \epsilon_t$$

(8)
$$\epsilon_t \sim \mathcal{N}(0, \sigma_t^2 + \sigma_J^2),$$

where θ_i is the vector of the orbital parameters of planet i, f is a periodic function as defined in Eq. 1 of (Wright and Howard, 2009), and σ_t is the nominal error bar on the measurement at time t. The free parameters are $n, c_0, \sigma_J, (\theta_i)_{i=1..n}$. We assume that there are at most $n_{max} = 3$ planets. We fix uninformative priors, which we do not specify for the sake of brevity, as they

¹An example of FIP calculation in Python is given here https://github.com/nathanchara/FIP.

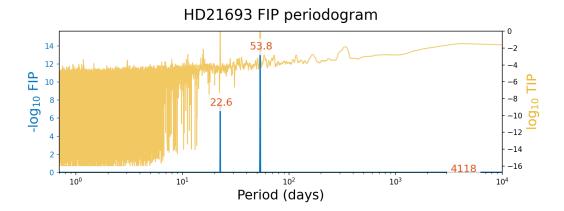


FIG 1. In blue: $-\log_{10}$ FIP of having a planet with frequency in interval $[\omega_k - \Delta\omega/2, \omega_k + \Delta\omega/2]$ as a function of ω_k for the HARPS data of HD 20003 (Udry et al., 2019) and a maximum of 2 planets. In yellow, we represent the true inclusion probability, TIP = 1-FIP.

do not matter here. The posterior distributions and Bayesian evidences are computed with the nested sampling algorithm POLYCHORD, (Handley, Hobson and Lasenby, 2015a,b).

As in Hara et al. (2022a); Toulis and Bean (2021), we consider that a planet has been correctly detected the period of the claimed planet is close to a true period with a certain accuracy. In the formalism of section 3.1, we choose the sets Θ_i s as frequency intervals of fixed length, chosen from a grid. The interval k of the grid is defined as $[\omega_k - \Delta\omega/2, \omega_k + \Delta\omega/2]$, where $\Delta\omega = 2\pi/T_{\rm obs}$, $T_{\rm obs}$ is the total observation time span, and $\omega_k = k\Delta\omega/N_{\rm oversampling}$. We take $N_{\rm oversampling} = 5$. For each interval in the grid, we compute the marginal probability to have a planet whose frequency lies in the interval, and its FIP as defined in Eq. (4)². The value of $-\log_{10}$ FIP as a function of frequency is represented in Fig. 1, and is called a FIP periodogram.

In the following sections, we show that the optimal detection procedure simply consists in claiming the detection of all signals with increasing FIP until a certain threshold is attained (see section 5.1). Here, for any reasonable FIP threshold, 0.01%-10%, two planets are detected. Indeed, the probability that there are no planets with frequencies $2\pi/53.8 \pm \Delta\omega$ rad/day and $2\pi/22.67 \pm \Delta\omega$ rad/day period is supported with FIP less than 10^{-6} . The interval with the third highest probability occurs at 4118 days, it has a FIP greater than 90%, and likely stems from low frequency noise.

3. Maximum utility. We want to minimise both false and missed detections, which is an optimisation problem that we first formalise in the utility framework (von Neumann and Morgenstern, 1947). In this one, a set of possible actions \mathcal{A} is defined, as well as a utility function U,

$$a \in \mathcal{A}, (\theta, \eta) \in \Theta \to U\{a, (\theta, \eta)\} \in \mathbb{R},$$

quantifying the gain of taking action a while the true value of the parameters of the patterns and the nuisance parameters are $\theta = (\theta_i)_{i=1,\dots,n}$ and η , respectively. The maximum utility action a^* , if it exists, is defined as maximizing the expectancy of the utility taken on the

²It is in fact more computationally efficient to loop over the samples and determine in which frequency interval they lie, see the Python example https://github.com/nathanchara/FIP.

posterior distribution of the pararameters,

(9)
$$a^{\star} = \arg \max_{a \in \mathcal{A}} E_{\theta, \eta} \left[U \left\{ a, (\theta, \eta) \right\} \right] = \int U \left\{ a, (\theta, \eta) \right\} p(\theta, \eta \mid y) \, \mathrm{d}\theta \, \mathrm{d}\eta.$$

We must choose the space of actions A and the utility function U for our problem. We choose

$$\mathcal{A} = \{a(\Theta_1, ..., \Theta_n), (\Theta_i)_{i=1...n} \in \mathcal{T}\}$$

where $a(\Theta_1,...,\Theta_n)$ is given in Definition 2.1. The action is unequivocally defined by the choice of $(\Theta_i)_{i=1...n} \in \mathcal{T}$, as a consequence, \mathcal{A} and \mathcal{T} can be identified.

3.1. Defining the utility function. We adopt the definition of false and missed detections given in Section 3.1, and we assign the value 0 to the utility if all the detections are correct. Each false detection has a cost $\alpha > 0$, and a missed detection has a cost $\beta \geqslant 0$. Denoting by $E[\mathrm{FD}]$ and $E[\mathrm{MD}]$ the expected number of false detections and missed detections when choosing $(\Theta_i)_{i=1...n}$, the expected utility is $-\alpha E[\mathrm{FD}] - \beta E[\mathrm{MD}]$. It is unnecessary to keep both α and β as parameters, and we will write utilities as a function of the relative cost of missed and false detection, $\gamma = \beta/\alpha$. We show in Appendix A that depending on whether we define missed detections as in Definition 2.3 or 2.4, the expected utility is either

(10)
$$E_{\theta,\eta} \left[U \left\{ a(\Theta_1, ..., \Theta_n), (\theta, \eta) \right\} \right] = -n + \sum_{j=1}^n j I_{A_j} - \gamma \sum_{k=n+1}^{n_{\text{max}}} (k-n) p(k \mid y),$$

or

(11)
$$E_{\theta,\eta}\left[U\left\{a(\Theta_1,...,\Theta_n),(\theta,\eta)\right\}\right] = -n + (1+\gamma)\sum_{j=1}^n jI_{A_j} - \gamma\sum_{k=1}^{n_{max}} kp(k\mid y).$$

where $p(k \mid y)$ is defined in Eq. (5) and I_{A_j} is the probability that exactly j detections are correct.

The expected utility is a function of $(\Theta_i)_{i=1..n}$, and we want to maximize it. To do so, we first maximize it with a fixed number of patterns n, then find the optimal n. For both definitions (10) and (11), maximizing the expected utility for a fixed n is equivalent to finding the $(\Theta_i^n)_{i=1..n}$ maximizing $\sum_{j=1}^n j I_{A_j}$, provided they exist. A priori, for $n' \neq n$ the optimal $(\Theta_i^n)_{i=1..n}$ and $(\Theta_i^{n'})_{i=1..n'}$ do not necessarily have something in common. As we shall see in the following, simplifications occur if the Θ_i s are "separable" in some sense.

3.2. Patterns with parameters in disjoint regions. A first simplification occurs if we restrict the search to Θ_i , i=1...n that are pairwise disjoint. One possible justification is that the physics forbids two patterns to occupy the same Θ_i .

LEMMA 3.1. Let us consider $\Theta_1 \in T, ..., \Theta_n \in T$, $\forall i_1, i_2 = 1...n, i_1 \neq i_2, \Theta_{i_1} \cap \Theta_{i_2} = \emptyset$. Then with I_{Θ_i} as defined in Eq. (2), and I_{A_i} as defined in Eq. (10)

(12)
$$\sum_{j=1}^{n} j I_{A_j} = \sum_{i=1}^{n} I_{\Theta_i}$$

The proof, given in Appendix B, simply uses a decomposition of the terms of the lefthand sum. The quantity I_{Θ_i} , the posterior probability to have a pattern in a space Θ_i , can be computed as explained in Section 2. If Eq. (12) is verified, adopting the definition of FIP of Eq. (4), maximising the utility (Eq. (10) or Eq. (11)) for a fixed number of patterns n comes down to solving

 (P_n)

$$(\Theta_i^n)_{i=1..n} = \arg\min_{\Theta_1 \in T, \dots, \Theta_n \in T, \Theta_i \cap \Theta_j = \emptyset} \sum_{i=1}^n \text{FIP}_{\Theta_i} = \arg\max_{\Theta_1 \in T, \dots, \Theta_n \in T, \Theta_i \cap \Theta_j = \emptyset} \sum_{i=1}^n I_{\Theta_i}.$$

We just want to find $(\Theta_i^n)_{i=1..n}$ maximizing the probability that they "host" a pattern. Note that lemma 3.1 is not true if the Θ_i s are allowed to have non empty intersection. This is easily seen for n=2, where $I_{A_1}^1=I_{\Theta_1\cup\Theta_2}^1$ which might not be equal to $I_{\Theta_1}^1+I_{\Theta_2}^1$ if Θ_1 and Θ_2 are not disjoint. In Appendix C we exhibit some conditions guaranteeing the existence of the solution to (P_n) , and now try to find it.

3.3. Searching for the optimum. To solve (P_n) for n=1, we simply need to find the region of the parameter space Θ^1_1 with maximum $I_{\Theta^1_1}$. It is tempting to build the solution for higher n from there. Supposing that (P_n) has a solution $(\Theta_i)_{i=1...n}^n$, a natural candidate solution for (P_{n+1}) is to append the space with maximum marginal probability outside the Θ^n_i s, which we denote by

$$\Theta_{n+1}^{\star} = \arg \max_{\Theta_{n+1} \in T \setminus \bigcup_{i=1}^{n} \Theta_{i}^{n}} I_{\Theta_{n+1}} = \arg \min_{\Theta_{n+1} \in T \setminus \bigcup_{i=1}^{n} \Theta_{i}^{n}} \operatorname{FIP}_{\Theta_{n+1}}.$$

The following result, proven in Appendix D, shows that this simple procedure is not always optimal.

LEMMA 3.2. Let us suppose that (P_n) has a solution $(\Theta_1^n,...,\Theta_n^n) \in \mathcal{T}$. Then the solution to (P_{n+1}) is either $(\Theta_1^n,...,\Theta_n^n,\Theta_{n+1}^*)$ or such that $\forall i=1...n+1, \exists j=1...n, \Theta_i^{n+1}\cap\Theta_j^n\neq\emptyset$.

Informally, the solution to (P_{n+1}) either consists in appending Θ_{n+1}^{\star} , or in arranging n+1 regions all intersecting at least one of the $(\Theta_i^n)_{i=1,\dots,n}$. In the example of Section 2.3, we wanted to determine the presence of a planet in a frequency interval of size $\Delta\omega=2\pi/T_{\rm obs}$, the frequency resolution dictated the total timespan of the observations $T_{\rm obs}$. Had we chosen a much smaller $\Delta\omega$, when searching for the solution to (P_n) with increasing n, the first interval chosen would be "glued" together to form a wider interval, capturing enough probability mass around the -logFIP modes. In this example and elsewhere, such iterative "gluing" essentially means that the Θ_i s do not capture the resolution provided by the likelihood, they are too small. Lemma 3.2 motivates the definition of separability, simply expressing the condition under which it can be ensured that the solution to (P_{n+1}) is to append Θ_{n+1}^{\star} (Eq. (13)).

DEFINITION 3.3 (Separability). We say that a dataset y verifies pattern separability of order $n \ge 2$ if (i) the solution to (P_{n-1}) , Θ_1^{n-1} ,..., Θ_{n-1}^{n-1} are pairwise disjoint and (ii) the solution to (P_n) is $(\Theta_1^{n-1},...,\Theta_n^{n-1},\Theta_n^{\star})$ as defined in Eq. (13). By convention we say that pattern separability is true at order 0 and 1.

If T is a metric space, separability is ensured as long as in the vicinity of the Θ_i s, the probability of having a signal is sufficiently low. We denote by $B(\theta, R)$ a closed balls of centre θ and radius R. In Appendix D we prove the following result.

LEMMA 3.4. Let us suppose that \mathcal{T} is the set of 0 to n_{\max} disjoint balls of radius R and centres $(\theta_i)_{i=1...n}$. Denoting by $\Theta^c = \bigcup_{i=1}^n B(\theta_i, \mathbf{3}R) \setminus \bigcup_{i=1}^n \Theta_i$, if $I_{\Theta^c} < I_{\Theta_{n+1}^*}$, then the patterns are separable of order n+1.

In the case considered in Section 5.3, we want to localise the period of exoplanets. Lemma 3.4 means that if the grid of intervals has width $\Delta\omega=2R$, and the prior excludes two planets being closer than $2\Delta\omega$, the separability condition is verified. There is one caveat to this assumption, which is the potential presence of co-orbital planets, sharing the same orbit (e.g Gascheau, 1843). To address that case, it is possible to either adopt the general formalism of section 3.1, or to further specify the Θ_i spaces to ranges of orbital frequencies and phase. The prior would exclude having two planets with parameters within the same Θ_i , as the system would be dynamically unstable.

4. Minimum missed detections under constraints. In section 3, we minimised the number of missed and false detections with a cost function. Alternatively, we can consider the following problem: among the possible choices of $n, (\Theta_1, ... \Theta_n)$ such that the expected number of false detections is lower than a certain $x \in [0, n_{\max}]$, which choice minimises the number of missed detections? For the definition of missed detections adopted in Definition. 2.3, this problem writes

(14)
$$\arg\min_{(n,\Theta_1,..\Theta_n)} \sum_{k=n+1}^{n_{\max}} (k-n) p(k\mid y) \text{ subject to } n-\sum_{j=1}^n j I_{A_j} \leqslant x.$$

Among the solutions to this problem, we further select the ones that minimise the term $n - \sum_{j=1}^{n} j I_{A_j}$. The rationale is that, for a given value of the objective function, there is no reason to select a solution with a higher expected number of false detection than necessary. For the Definition. 2.3 the constrained problem is

(15)
$$\arg\min_{(n,\Theta_1,..\Theta_n)} \bar{n} - \sum_{j=1}^n jI_{A_j} \text{ subject to } n - \sum_{j=1}^n jI_{A_j} \leqslant x,$$

where $\bar{n} = \sum_{k=1}^{n_{max}} kp(k \mid y)$ does not depend on $(\Theta_i)_{i=1,\dots,n}$. Maximising Eqs. (10) or (11) is similar to a "Lagrange multipliers" version of Eqs. (14) and (15). A natural question is whether the solutions of (14) and (15) obtained as x skims $[0, +\infty)$ also maximize Eqs. (10) and. (11), respectively, when γ skims $[0, +\infty)$. The following theorem shows that it is true if we have pattern separability as in Definition 3.3.

THEOREM 4.1. Let us consider a dataset y and suppose that it verifies pattern separability at all orders, $n=1...n_{\max}$ then there exists an increasing function $\gamma(x)\geqslant 0$ such that (10) and (14) have the same solution, and a function $\gamma'(x)\geqslant 0$ such that (11) and (15) have the same solution.

The detailed proof of is given in Appendix E, and relies on the following idea. Defining u_n and v_n the expected number of false and missed detection when solving (P_n) , we prove that u_n is increasing and v_n is decreasing. Thus, solving the constrained problem consists in finding n_0 , the maximum n such that $u_n < x$. Denoting by $\Delta u_n = u_n - u_{n-1}$, $\delta v_n = v_{n-1} - v_n$, and $w_n = \Delta u_n/\delta v_n$, writing the utility $u_n + \gamma v_n$, we see that provided we can choose a $\gamma(x)$ in between w_{n_0} and w_{n_0+1} , the maximum utility problem has the same solution as the constrained one. Now, we prove that under pattern separability, Δu_n and δv_n are increasing and decreasing, thus w_n is increasing and choosing an appropriate $\gamma(x)$ is possible. Furthermore, w_{n_0} is an increasing function of n_0 , which is an increasing function of x, so $\gamma(x)$ is an increasing function of x.

5. Discussion. Our initial aim was to find an optimal procedure to determine which parametric patterns are in the data in the framework described in section 2. We now discuss the final optimal procedure, when it is applicable, how it performs compared to other criteria and how it relates to other approaches.

5.1. Procedure. We considered two formulation of optimality: the maximum utility decision and minimum expected number of missed detection under a constraint on the expected number of false detections. We have seen in section 4 that the two are equivalent, provided a technical condition is satisfied (see Definition 3.3). If it is, suppose we have found the solution $(\Theta_i^n)_{i=1,\dots,n}$ solving (P_n) , that is maximizing the utility with n patterns. The maximum utility with n+1 patterns is obtained by appending Θ_{n+1}^{\star} , the space with minimum FIP outside the $(\Theta_i^n)_{i=1,\dots,n}$, as defined in Eq. (13). For the missed detections Definition 2.3, from Eq. (10), the n+1 pattern model has a greater utility than the n pattern model if and only if

(16)
$$\operatorname{FIP}_{\Theta_{n+1}^{\star}} \leqslant \gamma p(k \geqslant n+1 \mid y).$$

and we add patterns until this criterion is violated. It is not surprising that the marginal probability of having a pattern in a certain region appears, since it is the probability of the event of interest, which is consistent with a "Dutch book" principle (Ramsey, 1926; De Finetti, 1937).

Eq. (16) means in particular that, for a given γ , the more patterns are claimed, the more stringent the criterion to add a pattern becomes, since the term $p(k \ge n+1 \mid y)$ gets smaller as n increases. This contrasts with decisions based on a fixed threshold, for instance selecting a model with a Bayes factor greater than 150 (Kass and Raftery, 1995). However, if we now use the definition of missed detection 2.4, the n+1 pattern model has a greater utility than the n pattern model if and only if

(17)
$$\operatorname{FIP}_{\Theta_{n+1}^{\star}} \leqslant \frac{\gamma}{\gamma + 1},$$

which expresses the intuitive idea of a bet " γ to one". If the cost of missing a detection is γ when the cost of a false one is 1, then the FIP of the new signal should be less than $\gamma/(\gamma+1)$.

Typically, we would choose γ small to penalize false detections more than missed ones, and $\gamma/(\gamma+1)\sim\gamma$. In that case, the criterion of Eq. (16) is more stringent than the criterion of Eq. (17). This behaviour is to be expected, because in the second case, the utility function has an extra penalization of missed detections.

In the maximum utility case, one must know the maximum number of patterns possible $n_{\rm max}$, and be able to compute the Bayesian evidence up to that number, which might be computationally heavy or even intractable. To avoid computing Bayesian evidences for high dimensional models, we suggest to compute the FIPs each time $n_{\rm max}$ is incremented, until the FIPs of the candidate signals do not vary. This procedure is described in detail in the case of exoplanets in Hara et al. (2022a).

5.2. Applicability. Our formalism requires to choose the space \mathcal{T} , that is the possible choices of Θ_i s (see definition 2.1). If T is a metric space, we recommend to choose Θ_i s as balls of radius R. If the prior probability to have patterns with parameters θ_1 and θ_2 with $|\theta_1 - \theta_2| < 2R$ is vanishing, then one can search solutions to (P_n) without loss of generality.

Another important question is whether the separability condition 3.3 applies, in which case one can simply follow the procedure of Section 5.1. Thanks to Lemma 3.4, if the Θ_i s are chosen as balls of fixed radius it is easy to verify that the signal is indeed separable at order n+1, and ensure that appending Θ_{n+1}^* to the solution of (P_n) solves (P_{n+1}) . In practice, the value of R can always be chosen small enough to verify the separability condition, unless there can be patterns with exactly the same parameters. If such situation happens, it likely means that the Θ_i should be redefined. For instance, parametric descriptions of patterns typically include an amplitude, and the superposition of two identical patterns has simply twice the original amplitude. If simplifications are not possible, one can maximise utility in the general case (see Eq. (10) and (11)).

In our framework, the candidate Θ_i spaces in \mathcal{T} might have different sizes. If it is the case, the maximisation will favour larger Θ_i spaces. To prevent this situation, one can either fix the

TABLE 1
Priors used to generate and analyse the 1000 systems with circular orbits.

Parameter	Prior	Values
k	Uniform $[k_{\min}, k_{\max}]$	$k_{\min} = 0, k_{\max} = 2$
A	$egin{aligned} \mathcal{N}(0,\sigma_A^2) \ \mathcal{N}(0,\sigma_B^2) \ \mathcal{N}(0,\sigma_C^2) \end{aligned}$	$\sigma_A=1.5~\mathrm{m/s}$
В	$\mathcal{N}(0, \sigma_B^2)$	$\sigma_B=1.5~\mathrm{m/s}$
C	$\mathcal{N}(0, \sigma_C^2)$	$\sigma_C=1$ m/s
P	log-uniform on $[P_{\min}, P_{\max}]$	$P_{\min} = 1.5, P_{\max} = 100$

size of the Θ_i s, or add a penalisation term to Eq. (10) for the size of the Θ_i , for instance, by choosing a certain measure on T and adding a term $-\sum_i \mu(\Theta_i)$ to Eqs. (10) and (11). We leave this latter approach for future work.

5.3. Example. To show how the selection criterion (16) performs compared to other significance metrics, we apply it to the detection of sinusoidal signals in unevenly sampled data, where a certain precision on the frequency is desired. We use the simulations of Hara et al. (2022a) that emulate a search for exoplanets with radial velocity. The data are thus in velocity units (m/s).

Our goal is to evaluate different detection methods, provided the model used is correct. As a consequence, we analyse the data with the priors and likelihoods used to generate it. The procedures corresponding to Eqs. (16) and (17) are labelled Max. utility and FIP, respectively. We also test the best standard practices of the exoplanet communities. These procedures all proceed in two steps: finding candidate periods and assessing their statistical significance. To find the period, we use either a periodogram as defined in (Delisle, Hara and Ségransan, 2020a), a FIP periodogram as described in Section 2.3, using all the perior posterior, or a ℓ_1 periodogram, aiming at retrieving a sparse Fourier spectrum (Hara et al., 2017). The significance is either assessed with a false alarm probability (Delisle, Hara and Ségransan, 2020a), a Bayes factor defined as $p(y \mid k+1)/p(y \mid k)$ with $p(y \mid k)$ and false alarm probability (FAP) as defined in Eq. (6)) (Gregory, 2007), or taking the number of planets k maximising the posterior number of planets (PNP), $p(k \mid y)$. The detail of the different methods are given in Appendix F.

To evaluate the performance of the different analysis methods, if the frequency of a detected signal is more than $2\pi/T_{\rm obs}$ away from the frequency of a signal injected, it is considered as a false detection. If we claim n planets but there are n'>n we count n'-n missed detections. In other words, we adopt the definition of false and missed detection of Definitions 2.2 and 2.3, respectively. Therefore, we expect that the detection criterion (16) should perform slightly better than criterion (17). In Fig. 2 (a) and (b), we show the total number of mistakes for the high and low SNR simulations, respectively, made with the maximum utility criterion as a function of $\log_{10}\gamma$. It appears that the minimum number of mistakes is attained around $\log_{10}\gamma\sim0$ that is $\gamma\sim1$, that is when the missed and false detections are weighted equally.

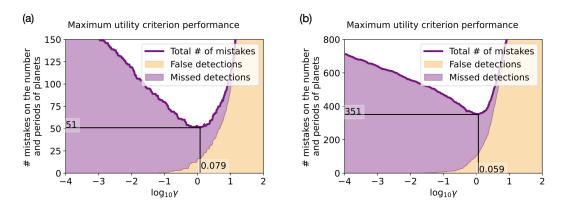


FIG 2. Missed + false detections, in yellow and purple respectively, as a function of the detection threshold, $\log_{10} \gamma$ where γ is defined in Eq. (16). (a) is obtained on the high SNR simulation and (b) the low SNR simulation. The black plain lines show where the minimum of mistakes is attained.

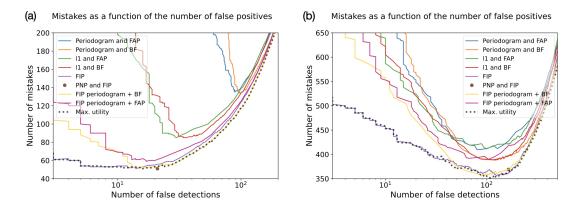


FIG 3. Missed + false detections as a function of the number of false detections for the different analysis methods. (a) and (b) are obtained on the high and low SNR simulations, respectively. The labels of the curves correspond to the methods used to find the candidate periods and to assess their significance. For instance, Periodogram and Bayes factor means that the candidate period is selected with a periodogram, and its significance assessed with a Bayes factor.

To compare the different detection methods, we compute the total number of mistakes as a function of the number of false detections, which vary as the detection threshold changes. In Fig. 3 (a) and (b) we show the curves obtained for the high and low SNR simulations, respectively. As expected, the FIP and maximum utility criterion outperform other metrics, notably in the low false positives regime, below ~ 10 , where it leads up to 30% more true detections than the alternatives.

As mentioned in section 1, our original concern was that existing methods de-couple the search for the period of the planet and its significance. In our numerical test, all the methods using the FIP periodogram select the candidate period exactly in the same way and differ only in the statistical significance metric. Our results confirm that, indeed, the scale of the significance metric has to be tied to the accuracy desired on the parameters, here on the period. In Hara et al. (2022a), we show that this is also the case in practice, through the analysis of the HARPS RV dataset of the star HD 10180 (Lovis et al., 2011).

5.4. Link with other approaches. Using a Bayesian decision-theoretic approach to test hypotheses has been done in other contexts. We discuss in particular the link of our approach with the Bayes factor, how to interpret posterior distributions when they are over spaces of several dimensions, and Bayesian false discovery rates.

- $5.4.1.\ Bayes\ factor\$. As mentioned in sections 1 and 5.3, the standard methodology to detect exoplanets is to compute the Bayes factor of n+1 versus n planet models. Bayes factor can also be seen in the framework of maximum utility (Bernardo and Smith, 2009). Assuming there are only two competing models, M_0 and M_1 , for i=0,2 the utility function is 1 if M_i , is selected and, is the true model, and 0 if it is not. This informs us on why the FIP might outperform the Bayes factor for locating patterns. The Bayes factor obliterates the fact that there can be more than n+1 or less than n planets. Suppose there are three planets in the data. Even if the candidate period is selected with the full marginal posterior, for instance a FIP periodogram, the estimate of the Bayes factor of 1 vs 0 planets will be sensitive to all the interferences of the three planetary signals. Even if the period of the candidate signal is appropriately estimated, the Bayes factor is not the most meaningful significance scale.
- 5.4.2. *Posterior re-labelling*. One of the problems that can occur when dealing with a posterior distribution across spaces of different dimensions, here, the number of patterns, is summarising the information contained in the posterior samples. In Roodaki, Bect and Fleury (2014), the authors define the notion of t-components, features that are present across dimensions. The FIP offers a way to establish such components, it essentially guarantees that some patterns are present, marginalising the posterior across several dimensions.
- 5.4.3. Bayesian false discovery rate. In Section 3.1 and 4, we respectively pose the problem in terms of maximisation of utility function and miminimum missed detections under constraint on the expected number of false one. Müller et al. (2004) uses the same definition of functions to optimize (they use loss functions instead of utility ones, which is strictly equivalent) in a different context: gene expression microarrays. In their case, they consider n different genes which might have an impact or not not the result of some experiment, and want to decide for gene i if it has a significant impact or not. In their parametrization, a variable z_i plays the role of the ground truth, $z_i = 0$ means the gene has no impact and $z_i = 1$, that it has. The optimal decision rule consists in selecting the the n^* genes with posterior probability of $z_i = 1$ greater than a certain threshold. They use this result to determine the appropriate sample size. Other works also consider discrete hypotheses, such as (Guindani, Müller and Zhang, 2009). Barbieri and Berger (2004) consider the problem where the data y are described by a linear model $y = Ax + \epsilon$, where each of the components of vector of size n, x, might be zero. They aim at finding the way to select the non zero components to have optimal predictive properties, and find that they must select the components with the probability to be non-zero greater than 1/2.

For our problem, we have to deal with a continuum of possibilities. If we choose the Θ_i as balls of fixed radius and centre θ , our hypotheses are indexed by the continuous variable θ . We can however adapt our framework to deal with the cases of Müller et al. (2004) by selecting T (see Section 2.1) as a discrete set of indices 1..n, and the case of Barbieri and Berger (2004) as the set of (i, θ_i) , where θ_i is a linear coefficient, i = 1, ..., n. We must further impose that the prior forbids to choose twice the same index, similarly to our separability condition (Definition 3.3).

With these choices, the result we would get using the formulation maximum utility function of Eq. (11), would be identical to Müller et al. (2004), but there could be a difference if we used the utility function of Eq. (10). Indeed, in Müller et al. (2004), the false negatives are considered as the indices that have wrongly not been selected, and the utility function Eq. (10) does not penalize these situations. They shown that the optimal detection criterion consists in selecting the n^* genes with a probability $P(z_i = 1 \mid y) > c/(c+1)$ where c controls

the relative cost of false positives and false negatives (in our formalism, $\gamma = 1/c$) which is exactly the same as Eq. (17).

In Muller, Parmigiani and Rice (2006), it is shown that the decision rule of Müller et al. (2004) based on a decision-theoretic approach has close links with Bayesian approaches to false discovery rate (FDR) (Efron et al., 2001) (see also Storey (2003); Scott and Berger (2006); Bogdan, Ghosh and Tokdar (2008); Stephens (2016)). The notion of FDR, introduced by Benjamini and Hochberg (1995) aims at controlling the proportion of false positives among the signals whose detection is claimed. As noted in Hara et al. (2022a), the FIP provides guarantees on the number of false detections. Indeed, among n statistically independent claims made with FIP = α , the number of false detections follows a binomial distributions of parameters α and n.

6. Model criticism. The optimal decision is chosen within a set of alternatives, which can be nested in a hierarchical structures. For instance, in the case of exoplanets there are many different ways to parametrize the noise due to the star (Aigrain, Pont and Zucker, 2012; Foreman-Mackey et al., 2017; Delisle, Hara and Ségransan, 2020b), whose respective Bayesian evidences can be compared (e.g. Ahrer et al., 2021). Instead of choosing a particular noise model, the FIP can simply be marginalised over the different noise models in a model averaging perspective. However, as noted in Rubin (1984), including models in increasingly deeper hierarchical structures has a computational limit. In Hara et al. (2022a), we showed numerically that the FIP exhibits a certain robustness to model misspecification, and here we aim to go further.

In the terms of Box (1980), we tackled the estimation problem (finding a decision in a set of alternatives), and now turn to the criticism problem: is the set of alternatives realistic? In the context of exoplanets, this latter problem is very seldom examined (Hara et al., 2019, proposes to run some tests on the residuals, which helps diagnosing whether the noise model is realistic).

Here, our priority is to gain confidence that our predictions are calibrated: statistically independent detections made with FIP = α should behave as independent Bernoulli variables with probability of success, when there is indeed a planet, of $1-\alpha$. Calibration is deemed desirable in different contexts: statistical inference (e.g. Box, 1980; Dawid, 1982; Rubin, 1984; Gneiting, Balabdaoui and Raftery, 2007; Draper and Krnjajic, 2010), predictions in a game-theoric setting (e.g. Foster and Vohra, 1998; Vovk and Shafer, 2005) and machine learning (e. g. Song et al., 2019). Even if the events which are assigned a probability may not be repeatable, the model (priors and likelihood) can be viewed as an "expert" which will take decisions repeatedly, and we want the expert to make calibrated predictions. If it is not the case, we want to understand which assumptions of the model are faulty.

6.1. General method. Calibration is often considered in a supervised manner: the truth can be known. For instance, when assessing the calibration of a method predicting the weather, it can be known for sure whether in fact it was sunny or rainy (e.g. Foster and Vohra, 1998; Vovk and Shafer, 2005). However, for exoplanets it cannot be ensured with certainty, and rarely with extremely high probability that a decision is correct. To circumvent this issue, we adopt the same Bayesian cross validation formalism as Vehtari and Lampinen (2002) (see also Draper and Krnjajic (2010)). The data y on which the inference is based, whenever possible, is divided in two. The first part (training set) is used to compute a posterior for the predictive distribution on the second part (test set), which is then compared to the actual data. For instance, if y is a time series $y(t_i)_{i=1..N}$, we can separate it in a training sets with $y_{\text{train}} = \{y(t_i), t_i < t_0\}$ and a test set $y_{\text{test}} = \{y(t_i), t_i > t_0\}$ for some threshold t_0 , and compare y_{test} to the distribution of what should be observed at times $t_{\text{test}} = t_i > t_0$, knowing y_{train} , which we denote by $p(y^* \mid y_{\text{train}})$.

Let us suppose we are able to generate realisations of y^* following $p(y^* \mid y_{\text{test}})$. We compute several statistics $T_i(y^*), i=1..p$, where each T_i retrieves a real number, and compare their distributions to $T_i(y_{\text{test}})$. In Vehtari and Lampinen (2002), such statistics are defined as utilities expressing the discrepancy between the predicted data and the actual one. To ensure the predictions are calibrated, we envision two possibilities. As in Gneiting, Balabdaoui and Raftery (2007), we can leverage that, denoting by F_X the cumulative distribution function of random variable X, $F_{T_i}^{-1}(T_i(y_{\text{test}}))$ should be distributed uniformly on [0,1]. Second, we can define $T_i(y^*)$ as Bernoulli variables with probability of success, $T_i(y^*)=1$, equal to p_i . The total number of successes on the n is on average $\sum_{i=1,...,n} p_i$. If the T_i s are chosen to be independent, the number of successes follows a Binomial distribution, otherwise the distribution can be estimated with the empirical joint distribution of $(T_i(y^*))_{i=1,...,n}$, obtained from the different realisations of y^* following $p(y^* \mid y_{\text{test}})$. As a remark, the number of relevant tests is limited by the Data processing inequality (Cover and Thomas, 2006), $I((T_i(y^*))_{i=1,...,n}; y) \leqslant I(y^*; y)$, where I is the mutual information.

The prior predictive test proposed by Box (1980) is a particular case of our cross-validation test when the training set is the empty set, and the statistic considered is the Bayesian evidence. The posterior predictive test of Rubin (1984); Gelman, Meng and Stern (1996), conveys the idea that, if the exact same experience was to be repeated, we would want the actual observations not to be too improbable an outcome, and chooses $y_{\text{test}} = y_{\text{train}} = y$.

To assess the calibration of our detections, we want to express that if a pattern has been detected in the training set, it should still be present in the test set. A natural way to define the statistics would be to determine on y_{train} the sets $\Theta_i \subset T, i=1,...,n$ maximizing the utility. Suppose we draw y^* from the predictive distribution. Conditioning on y^* , we obtain posterior probabilities to have planets in each Θ_i , $p_i(y^*)$, which can be our statistics $T_i(y^*) = p_i(y^*)$. Now as y^* follows the predictive distribution $p(y^* \mid y_{\text{train}})$, we obtain samples of the posterior distribution of $p_i(y^*)$. Unfortunately, such calculations would in general require to evaluate $p_i(y^*)$ for many realizations of y^* . At least for exoplanets, this is unrealistic. Furthermore, these statistics alone does not allow to diagnose which assumptions of the model should be changed. How the data should be split, and which statistics to choose are difficult questions, and should be decided on a case by case basis.

6.2. Example. In the case of radial velocities, we suggest to define the statistics T_i based on the Fourier transform (or periodogram) of the predicted data. To illustrate this, let us suppose that conditioned on a time series y_{train} , at times t_{train} , the predictive distribution of data acquired at times t_{test} , $p(y^* \mid y_{\text{train}})$, is such that we can draw samples from it as

(18)
$$y^{\star}(t_{\text{test}}) = A\cos\omega t_{\text{test}} + B\sin\omega t_{\text{test}} + \epsilon$$

where A, B, ω are drawn from their posterior distribution knowing y_{train} , which are assumed to be Gaussian distributions of mean and standard deviation $\mu_A, \sigma_A, \mu_B, \sigma_B$ and $\mu_\omega, \sigma_\omega$ respectively. We further assume that ϵ is a homoskedastic Gaussian noise of zero mean and standard deviation σ .

We can define the test statistic as a Bernoulli variable, $T_1(y^*)=1$ if the modulus of the Fourier transform of y^* at frequency μ_ω is within certain bounds, and 0 otherwise. This expresses the idea that the putative planetary signal is still present. We can also define a series of test $T_i(y^*)=1$ if the amplitude of the Fourier transform of y^* at frequency $\omega_i, i=1,...,p$ is within certain bounds. This conveys the idea that the noise spectrum should be flat.

To fix ideas, we take $t_{\rm test}$ as a hundred equispaced measurements, assuming that they are taken each day. We generate 100,000 realisations of y^* according to Eq. (18), and compute the centred 90% credible intervals of each Fourier coefficient of y^* . In Fig. 4 (a), points show the absolute values of the Fourier coefficient for one of the 100,000 realisations. Four out

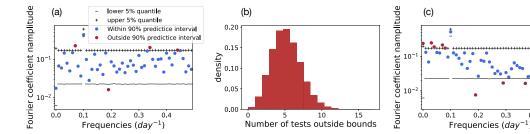


FIG 4. In (a) and (c) we show with markers - and + the bounds of the intervals where the modulus of Fourier coefficients should be as a function of frequency. Points represent the modulus of Fourier coefficients of a certain realisation of predicted data. Points inside and outside the 90% interval bounds are shown in blue and red, respectively. Figures (a) and (c) correspond respectively to a realisation of the predictive distribution, and a Gaussian stationary noise with an exponential autocorrelation $e^{-\Delta t/\tau}$ with a timescale $\tau = 3$ days. Figure (b) represents the histogram of the numbers of Fourier moduli outside bounds obtaines with the 100,000 realisations of the predictive distribution.

of a hundred coefficients are outside of the 90% intervals. Because of random fluctuations, we expect a stochastic variation of the number of coefficients outside bounds. In Fig. 4 (b), we show the distribution of the number of the number of coefficients outside bound, and four is not unusual. Let us now compute the absolute values of the Fourier coefficients of a realisation of y^* such that instead of generating white noise of variance 1 m^2/s^2 on top of a planetary signal, we generate a correlated Gaussian stationary noise with an exponential autocorrelation $e^{-\Delta t/\tau}$ with a timescale $\tau = 3$ days, such that the diagonal has also a variance of 1 m^2/s^2 . In that case, we find as expected higher and lower amplitudes at low and high frequency respectively, and twelve tests are outside of bounds.

To refine our tests, we can take as statistics the amplitudes of the putative planets fitted with a noise model, and the amplitudes of the Fourier transforms of the noise after fitting the planetary signals. The predicted phase of the putative planets can be examined, which offers an alternative to the phase consistency tests of Hara et al. (2022b).

7. Conclusion. Our initial aim was to find which parametric patterns are present in a dataset. We assume that there are n=0 to n_{\max} patterns, with parameters $(\theta_i)_{i=1...n} \in T^n$ for some space T, and there are nuisance signals parametrized by η . For data y, we assume that a likelihood $p(y \mid n, (\theta_i)_{i=1...n}, \eta)$ has been defined as well as proper priors on $n, (\theta_i)_{i=1...n}, \eta$. We considered detection claims of the form: "there are n patterns, one with parameters in Θ_1 , ..., one with parameters in Θ_n " where the Θ_i s are regions of the parameter space belonging to a predefined family of alternatives. For each i such that there is no such pattern truly with parameters in Θ_i , we count a false detection. Conversely, underestimating the number of patterns or not finding true ones corresponds to missed detections. This formulation requires to choose the candidate regions Θ_i . If T is a metric space, we recommend to choose a set of the closed balls of fixed radius R, which fixes the resolution desired on the pattern parameters. If possible, we recommend to choose R such that two patterns cannot be closer than 2R.

7.1. General case. We found that essentially, provided the patterns cannot have parameters too close to each other, which we formalise as the separability condition 3.3, the optimal detection procedure consists in selecting the regions Θ_i with a sufficient posterior probability to "host" the parameters of a pattern. Depending on the exact definition of missed detections, the thresholds to adopt are (16) or (17), and our approach can be seen as an extension of Bayesian false discovery rate to continuous indices (see section 5). If the separability condition is not met, the problem can be solved with a more general formulation (see section 3). Our significance metric is a posterior probability, which is particularly meaningful if it is calibrated: detections made with probability α are correct on average in a fraction α of cases. We leverage this property to test whether the prior and likelihood chosen are realistic.

Both the optimal criterion discussed in sections 2-5 and the calibration discussed in Section 6, can be seen through an uncertainty principle. In the first case, the smaller the Θ_i s are chosen, the more resolution we have on the pattern parameters, but the less probability mass will be contained in the Θ_i s. Similarly, we might ensure calibration using the data of a whole survey (for example, several hundreds of stars observed with the same instrument), or we might want to ensure calibration on a subset of events: for detections around certain type of stars, detections of small planets etc. This restricts the number of tests that can be run, thus the statistical power of calibration tests.

From a theoretical perspective, the next step will be to determine an analytical approximation of the minimum expected number of missed detections under a constraint on expected number of false detections, as a function of the prior distribution of parameters and the likelihood. This way, it will be possible to predict the optimal capabilities of a survey operating at a certain precision, assuming a data model (a certain parametric form for the priors and likelihood).

7.2. Exoplanets and astronomy. For the detection of exoplanets with radial velocities, instead of using the Bayes factor to determine the number of planets, it is more advantageous to proceed as follows. We define $\Delta\omega=2\pi/T_{obs}$ where T_{obs} is the observational time-span, and a grid of tightly spaced frequencies ω_k which defines a collection of intervals $I_k=[\omega_k-\Delta\omega/2,\omega_k-\Delta\omega/2]$. One then simply has to compute the posterior probability to have a planet with frequency in I_k (TIP) or the FIP = 1-TIP. The next step is to select the maximum number n^* of disjoint intervals with a FIP satisfying either the condition (16) or see Eq. (17), which correspond to slightly different penalization of false negatives (see Eq. (10) and (11)). We recommend the latter for simplicity, which is simply taking the intervals with FIP lower than a certain threshold (see Hara et al. (2022a) for a practical example).

For other observational technique the procedure is the same. If a correct detection is defined as one of the parameters being in a certain region, one must compute the posterior probability to have a planet with parameters in this region marginalised on the number of planets. Additional work is needed to make our framework computationally tractable for transits, imaging and microlensing, where datasets are typically much more voluminous. It will also be interesting to test the method in other contexts, such as the detection of gamma ray emissions (e.g. Geringer-Sameth et al., 2015).

To detect exoplanets, different models are compared to each other (different number of planets, different noise models). The present work gives a criterion with optimality properties once a set of alternative models have been considered. So far, whether the ensemble of alternatives considered is plausible, or if all the alternatives are poor, is almost never addressed. In Section 6, we propose a method to tackle this question, based on the predictive distribution. Such tests are to be refined in future work.

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APPENDIX A: EXPRESSION OF THE UTILITY FUNCTION

In this appendix, we show how to obtain the expression of the utility function (10). We make a detection claim as in Definition 2.1), and penalise false and missed detections as described in Section 3.1. Let us first compute the utility function for the claim "there is no pattern", denoted by a_0 .

(19)
$$E_{\eta}\{U(a_0,\eta)\} = 0 \times p(0 \mid y) - \beta \sum_{k=1}^{n_{max}} kp(k \mid y).$$

If in fact there are k patterns, we "pay" $k\beta$, hence the $-\beta \sum_{k=1}^n kp(k\mid y)$ term, where $p(k\mid y)$ the posterior probability of having k patterns.

When claiming the detection of n > 0 patterns with parameters in Θ_i , i = 1...n, the Θ_i s can be considered as n "boxes". We want to evaluate the utility of this claim if the true patterns have parameters $\theta_1, \dots, \theta_k$, where k might be different from n. We consider ways to put the θ_i in the boxes such that each θ_i can go into only one "box". Thus, if one of the θ_i is such that θ_i belongs to several Θ_i , we consider that only one pattern has been found. We denote by m the maximum number of different θ_i s that we can put in a Θ_i . We denote by A_m^k the region of parameter space with k patterns such that there is exactly one pattern in each of the Θ_i , i = 1..m, $m \leq n$.

(20)
$$E_{\theta,\eta}[U\{a,(\theta,\eta)\}] = -n\alpha p(0 \mid y)$$

(21)
$$+ \left[-(n-1)\alpha I_{A_1^1} - n\alpha \left(1 - I_{A_1^1} \right) \right] p(1 \mid y)$$

$$(22) \qquad + \left[-(n-2)\alpha I_{A_2^2} - (n-1)\alpha I_{A_1^2} - n\alpha \left(1 - I_{A_1^2} - I_{A_2^2} \right) \right] p(2 \mid y)$$

(23)

(24)
$$+ \left[\sum_{i=1}^{n} -(n-i)\alpha I_{A_{i}^{n}} - n\alpha \left(1 - \sum_{i=1}^{n} I_{A_{i}^{n}} \right) \right] p(n \mid y)$$

$$(25) \qquad + \left[\sum_{i=1}^{n} -(n-i)\alpha I_{A_{i}^{n+1}} - n\alpha \left(1 - \sum_{i=1}^{n} I_{A_{i}^{n+1}} \right) - \beta \right] p(n+1 \mid y)$$

(27)
$$+ \left[\sum_{i=1}^{n} -(n-i)\alpha I_{A_{i}^{n}} - n\alpha \left(1 - \sum_{i=1}^{n} I_{A_{i}^{n_{max}}} \right) - (n_{max} - n)\beta \right] p(n_{max} \mid y)$$

Re-arranging the terms, we have

(28)
$$E_{\theta,\eta}[U\{a,(\theta,\eta)\}] = -n\alpha + \alpha \sum_{i=1}^{n} iI_{A_i} - \beta \sum_{k=n+1}^{n_{max}} (k-n)p(k \mid y)$$

(29)
$$= -(\alpha E[FD] + \beta E[MD])$$

where E[FD] and E[MD] are the expected numbers of false detections and missed detections, respectively.

(30)
$$E[FD] = n - \sum_{i=1}^{n} iI_{A_i}$$

(31)
$$E[MD] = \sum_{k=n+1}^{n_{max}} (k-n)p(k \mid y)$$

Assuming that $\alpha \neq 0$ (or equivalently $\alpha > 0$, since α is non negative), we can divide Eq. (29) by α . Denoting by $\gamma = \beta/\alpha$, without loss of generality we can maximize

(32)
$$E_{\theta,\eta}\left[U\left\{a(\Theta_1,...,\Theta_n),(\theta,\eta)\right\}\right] = -n + \sum_{j=1}^n j I_{A_j} - \gamma \sum_{k=n+1}^{n_{max}} (k-n) p(k\mid y).$$

Alternatively, we can further penalize the missed detections. If k planets are truly present in the data, n detections are claimed but only i are correct, it means that the true detections of $\min(k,n)-i$ are missed. We can penalize this situation by adding a term $-\beta(\min(k,n)-i)$ whenever it happens. The expression of the utility function is now

(33)

$$E_{\theta,\eta}\left[U\left\{a,(\theta,\eta)\right\}\right] = -n\alpha p(0\mid y)$$

$$(34) + \left[-(n-1)\alpha I_{A_1^1} - (n\alpha + \beta) \left(1 - I_{A_1^1} \right) \right] p(1 \mid y)$$

$$+ \left[-(n-2)\alpha I_{A_2^2} - ((n-1)\alpha + \beta)I_{A_1^2} - (n\alpha + 2\beta) \left(1 - I_{A_1^2} - I_{A_2^2} \right) \right] p(2 \mid y)$$

(36)

:

(37)
$$+ \left[\sum_{i=1}^{k} (-(n-i)\alpha - (k-i)\beta) I_{A_i^k} - (n\alpha + k\beta) \left(1 - \sum_{i=1}^{k} I_{A_i^k} \right) \right] p(k \mid y)$$

(38)

:

(39)

$$+ \left[\sum_{i=1}^{n} -(n-i)(\alpha+\beta)I_{A_{i}^{n}} - n(\alpha+\beta) \left(1 - \sum_{i=1}^{n} I_{A_{i}^{n}} \right) \right] p(n \mid y)$$
(40)

$$+ \left[\sum_{i=1}^{n} -(n-i)(\alpha+\beta)I_{A_{i}^{n+1}} - n(\alpha+\beta) \left(1 - \sum_{i=1}^{n} I_{A_{i}^{n+1}} \right) - \beta \right] p(n+1 \mid y)$$
(41)

$$\vdots$$

$$+ \left[\sum_{i=1}^{n} -(n-i)(\alpha+\beta)I_{A_{i}^{n}} - n(\alpha+\beta) \left(1 - \sum_{i=1}^{n} I_{A_{i}^{n_{max}}} \right) - (n_{max} - n)\beta \right] p(n_{max} \mid y)$$

Re-arranging the terms, we have

(43)
$$E_{\theta,\eta} [U \{a, (\theta, \eta)\}] = -n\alpha + (\alpha + \beta) \sum_{i=1}^{n} iI_{A_i} - \beta \sum_{k=1}^{n_{max}} kp(k \mid y)$$

$$= -(\alpha E[FD] + \beta E[MD])$$

where E[FD] and E[MD] are the expected numbers of false detections and missed detections when claiming the detection of patterns with parameters in $\Theta_1, ..., \Theta_n$, respectively,

(45)
$$E[FD] = n - \sum_{i=1}^{n} iI_{A_i}$$

(46)
$$E[MD] = \bar{n} - \sum_{i=1}^{n} iI_{A_i},$$

where $\bar{n} := \sum_{k=1}^{n_{max}} kp(k \mid y)$ does not depend on the number of pattern claimed n. Again, re-normalizing by $\alpha > 0$

(47)
$$E_{\theta,\eta} [U \{a, (\theta, \eta)\}] = -n + (1+\gamma) \sum_{i=1}^{n} i I_{A_i} - \gamma \sum_{k=1}^{n_{max}} k p(k \mid y).$$

The sum on the right is simply the expectancy of k and does not depend on the number of planets.

APPENDIX B: PROOF OF LEMMA 1

Lemma B.1. Let us consider $\Theta_1 \in T, ..., \Theta_n \in T$, $\forall i_1, i_2 = 1...n, i_1 \neq i_2, \Theta_{i_1} \cap \Theta_{i_2} = \emptyset$. Denoting by A_i the subset of Θ such that there are exactly i patterns in $\Theta_1, ..., \Theta_n$, then

(48)
$$\sum_{j=1}^{n} j I_{A_{j}} = \sum_{i=1}^{n} I_{\Theta_{i}}$$

where I_{Θ_i} is defined in Eq. 2

We begin with a technical remark.

REMARK B.2. Since all patterns are interchangeable in the model, the ordering chosen between them is of no consequence. The detection claims are invariant by relabeling of the parameters, between different factors of T, i.e. having exactly one pattern in Θ_1 ,... exactly one in Θ_n is equivalent to having exactly one pattern in $\Theta_{\sigma(1)}$,... exactly one in $\Theta_{\sigma(n)}$ for any permutation σ of the n labels.

PROOF. Let us denote by $\Theta_1 \wedge \Theta_2 \wedge ... \wedge \Theta_j \backslash \Theta_{j+1}, ..., \Theta_n$ regions of Θ such that j patterns are in $\Theta_1, \Theta_2, ..., \Theta_j$ and no patterns are in $\Theta_{j+1}, ..., \Theta_n$. Then, since the Θ_i are disjoint, we can decompose I_{Θ_i} as a sum of posterior mass over regions that have a pattern in Θ_i but not other pattern in one of the Θ_j , $j \neq i$, regions that have a pattern in Θ_i and Θ_j but none in Θ_k , $k \neq i$, $k \neq j$ and so on.

$$I_{\Theta_i} = \sum_{j=0}^{n-1} \sum_{k_1, \dots, k_j \in [1, n]_j \setminus \{i\}} I_{\Theta_i \wedge \Theta_{k_1} \wedge \dots \wedge \Theta_{k_j} \setminus \Theta_{k_{j+1}}, \dots, \Theta_{k_n}}$$

where $[\![1,n]\!]_j$ is a draw of j indices without replacement in $[\![1,n]\!]$. For j=1..n,

(50)
$$I_{A_j} = \sum_{k_1, \dots, k_j \in [[1, n]]_j} I_{\Theta_{k_1} \wedge \Theta_{k_2} \wedge \dots \wedge \Theta_{k_j} \setminus \Theta_{k_{j+1}}, \dots, \Theta_{k_n}}$$

Then

(51)
$$\sum_{i=1}^{n} I_{\Theta_{i}} = \sum_{i=1}^{n} \sum_{j=0}^{n-1} \sum_{k_{1},\dots,k_{j} \in [[1,n]]_{j} \setminus \{i\}} I_{\Theta_{i} \wedge \Theta_{k_{1}} \wedge \dots \wedge \Theta_{k_{j}} \setminus \Theta_{k_{j+1}},\dots,\Theta_{k_{n}}}$$

In this sum, the term $I_{\Theta_1 \wedge \Theta_2 \wedge ... \wedge \Theta_n}$ appears n times, the terms $I_{\Theta_1 \wedge ... \wedge \Theta_{i-1} \wedge \Theta_{i+1} \wedge ... \wedge \Theta_n}$ appear n-1 times, so we obtain the desired result.

APPENDIX C: EXISTENCE OF THE SOLUTION

The existence of the solution to (P_n) can be guaranteed in the following situation. Let us suppose that T is a metric space, and let us denote by B_a a ball (closed or open) of fixed radius L in T centered on $a \in T$.

LEMMA C.1. Assume T is a finite dimensional Riemannian manifold (or more restrictively a finite product of \mathbb{S}^1 (angles) and \mathbb{R} (actions).) Let us suppose that $\mathcal{A} = \{B_{a_1},...,B_{a_n},k=1,...n_{max},a_1,...,a_k\in T_0^k\}$ where T_0 is a compact subset of T. Then the maximisation problem (P_n) has a (not necessarily unique) solution.

PROOF. Note first that if the posterior probability is regular enough (non-singular with respect to Lebesgue measure), which we assume, the problem consists in maximizing, for each n, a linear combination of integrals of this distribution over sets in \mathcal{A} . As the center a_i move continuously, the integration sets A_i move continuously (in the Hausdorff topology for instance), and integration over them is continuous. Thus we are maximizing a continuous functional.

Let us first show that the problem has a solution for each fixed n. The set of candidates is a smooth manifold, and the dependence of the functional to maximize is through integrating a probability distribution over sets of fixed diameters. As the centers a_i of the balls go to infinity, the probability distribution has to become very small, and so does its integrals over fixed-sized balls; thus the value of the function to maximize goes to 0 has the parameters go to infinity. Since the functional is positive and non-zero, there is some $\epsilon > 0$ such that the set on which the functional is bigger than ϵ is compact. The functional, being continuous, attains

its maximum on this set and this is then necessarily a global maximum. Then the maximum for $0 \le n \le n_{max}$ is a maximum of (P_n) . (Or if n is not bounded, the values of the integrals of the posterior distribution as a function of n have to decrease to 0 uniformly since the whole probability distribution sums to 1, so by the same argument as above the maximum is attained for bounded n.)

APPENDIX D: PROOF OF LEMMA 2

LEMMA D.1. Let us suppose that (P_n) has a solution $\Theta_1^n \in T, ..., \Theta_n^n \in T$, with $I_{\Theta_1^n} \geqslant$ $... \geqslant I_{\Theta_n^n}$. Then the solution to (P_{n+1}) is either $(\Theta_1^n,...,\Theta_n^n,\Theta_{n+1}^{\star})$ or such that $\forall i \in [1,n+1]$ 1]], $\exists j \in [1, n]$ such that $\Theta_i^{n+1} \cap \Theta_i^n \neq \emptyset$.

PROOF. The proof relies on the simple property (P1): if a function $f: E \to \mathbb{R}$ attains its maximum in a set X, then $\forall D \subset E$ such that $X \cap D = \emptyset$, the set of solution to arg $\max_{x \in E \setminus D} f(x)$ is X.

Let us consider $\Theta_{n+1} \in T$. The solution to (P_{n+1}) can be written as

(52)
$$\arg \max_{\substack{\Theta_1 \in T \setminus \Theta_{n+1}, \dots \Theta_n \in T \setminus \Theta_{n+1} \\ \forall i, j \in [\![1, n]\!], i \neq j, \Theta_i \cap \Theta_j = \emptyset}} I_{\Theta_{n+1}} + \sum_{i=1}^n I_{\Theta_i}.$$

Either $\forall i \in [1, n]$, $\Theta_{n+1}^{n+1} \cap \Theta_i^n = \emptyset$ then thanks to (P1), for $E = T^n$ and $D = \{x_1, ..., x_n \in \mathbb{R}\}$ $T^n, \forall i, x_i \notin \Theta_{n+1}^{n+1}$

(53)
$$\underset{\substack{\Theta_1 \in T \setminus \Theta_{n+1}, \dots \Theta_n \in T \setminus \Theta_{n+1} \\ \forall i, j \in [1, n], i \neq j, \Theta_i \cap \Theta_j = \emptyset}}{\max} \sum_{i=1}^n I_{\Theta_i} = (\Theta_i^n)_{i=1..n}$$

As a consequence,

$$(54) \ \arg\max_{\Theta_{n+1} \in T \setminus \bigcup_{i=1}^n \Theta_i^n} \arg\max_{\substack{\Theta_1 \in T \setminus \Theta_{n+1}, \ldots \Theta_n \in T \setminus \Theta_{n+1} \\ \forall i, j \in \llbracket 1, n \rrbracket, i \neq j, \Theta_i \cap \Theta_j = \emptyset}} I_{\Theta_{n+1}} + \sum_{i=1}^n I_{\Theta_i} = (\Theta_1^n, \ldots, \Theta_n^n, \Theta_{n+1}^\star)$$

up to a permutation of the indices (see remark B.2). If $\exists i \in [1, n+1], \forall j \in [1, n] \in \Theta_i \cap$ $\Theta_i^n = \emptyset$ then the same argument applies and the solution to (P_{n+1}) is $(\Theta_1^n, ..., \Theta_n^n, \Theta_{n+1}^{\star})$.

Let us denote by $\neg P$ the negation of a proposition P. Since $\neg(\exists i \in [1, n+1], \forall j \in [n+1], \forall$ $[\![1,n]\!], \Theta_i \cap \Theta_i^n = \emptyset) = \forall i \in [\![1,n+1]\!], \exists j \in [\![1,n]\!], \Theta_i \cap \Theta_i^n \neq \emptyset$, and the union of the two cases account for all cases, we obtain the desired result.

We now consider the case where T is a metric space and the Θ_i s are balls of fixed radius.

LEMMA D.2. Let us suppose that T is the set of 0 to n_{max} disjoint balls of radius Rand centres $(\theta_i)_{i=1...n}$. Denoting by $\Theta^c = \bigcup_{i=1}^n B(\theta_i, \mathbf{3}R) \setminus \bigcup_{i=1}^n \Theta_i$, if $I_{\Theta^c} < I_{\Theta_{n+1}^*}$, then the patterns are separable of order n + 1.

PROOF. Θ^c is the space described by any set of balls of radius R with a non empty intersection with the Θ_i , i=1...n. If $I_{\Theta^c} < I_{\Theta_{n+1}^*}$ there cannot be n+1 disjoint regions $(\Theta_i^{n+1})_{i=1...n+1}$ with non zero intersection with Θ_i , i=1...n with $\sum_{i=1}^{n+1} I_{\Theta_i^{n+1}} \geqslant$ $I_{\Theta_{n+1}^{\star}} + \sum_{i=1}^{n} I_{\Theta_{i}^{n}}.$

APPENDIX E: PROOFS OF THE RESULTS OF SECTION 4.2

In this appendix, we prove Theorem 4.1, which assumes pattern separability (Definition 3.3). This assumption is stronger than necessary for some of the lemmas, and is not made by default. However, we assume throughout the appendix that the Θ_i s are pairwise disjoint. Thanks to Lemma 3.1, using Eq. (4), we can write $n - \sum_{j=1}^n jI_{A_j} = \sum_{i=1}^n \mathrm{FIP}_{\Theta_i}$. We consider $\Theta_1^n, \ldots, \Theta_n^n$, solving (P_n) , and define

(55)
$$u_n := \sum_{i=1}^n \mathrm{FIP}_{\Theta_i^n}$$

(56)
$$v_n := \sum_{k=n+1}^{n_{\text{max}}} (k-n)p(k \mid y) \quad ; \quad {v'}_n = \bar{n} - n + \sum_{i=1}^n \text{FIP}_{\Theta_i^n}.$$

where $\bar{n} = \sum_{k=1}^{n_{max}} kp(k \mid y)$. The sequence u_n is the expected number of false detections, v_n and v'_n are the expected number of missed detections for the missed detection Definitions of 2.3 and 2.4, respectively (see Appendix A for details). Note that u_n , v_n and v'_n depend on y, but we chose not to make that dependence explicit to simplify notations.

LEMMA E.1. $\forall y$ in the sample space the sequence $(u_n)_{n=1..n_{max}}$ is increasing, $(v_n)_{n=1..n_{max}}$ and $(v'_n)_{n=1..n_{max}}$ are decreasing.

PROOF. Let us suppose that there exists n such that $u_{n+1} < u_n$. That is

(57)
$$n+1-\sum_{i=1}^{n+1}I_{\Theta_{i}^{n+1}} < n-\sum_{i=1}^{n}I_{\Theta_{i}^{n}}$$

This is equivalent to

(58)
$$1 + \sum_{i=1}^{n} I_{\Theta_i^n} < \sum_{i=1}^{n+1} I_{\Theta_i^{n+1}}$$

Let us denote by i_0 an index such that $i_0 = \arg\max_{i=1..n+1} I_{\Theta_i}^{n+1}$. Then

(59)
$$1 \leqslant 1 + \sum_{i=1}^{n} I_{\Theta_i^n} - \sum_{i=1, i \neq i_0}^{n+1} I_{\Theta_i^{n+1}} < I_{\Theta_{i_0}^{n+1}}$$

Where the left inequality stems from the definition of the Θ_i^n and Θ_i^{n+1} . Indeed, by definition $\sum_{i=1}^n I_{\Theta_i^n}$ is the maximum sum of probability mass on n disjoint Θ_i ,

(60)
$$\sum_{i=1}^{n} I_{\Theta_i^n} \geqslant \sum_{i=1, i \neq i_0}^{n+1} I_{\Theta_i^{n+1}}.$$

We then have $1 < I_{\Theta_{i_0}^{n+1}}$, which is absurd.

We have
$$v_{n+1} - v_n = -\sum_{k=n+1}^{n_{\max}} p(k \mid y) \leq 0$$
, and $v'_{n+1} - v'_n = u_{n+1} - u_n - 1 = \sum_{i=1}^n I_{\Theta_i^n} - \sum_{i=1}^{n+1} I_{\Theta_i^{n+1}} \leq 0$ by definition of Θ_i^n and Θ_i^{n+1} .

Because of this result, we can now ensure that the solution to the constrained problem is simply taking the maximum n for which the constraint is verified.

LEMMA E.2. If $(u_{n+1} - u_n)_{n=0..n_{\text{max}}}$ is increasing, there exists an increasing function $\gamma(x) \geqslant 0$ such that the solution maximising (10) solves the constrained problem (14) and an increasing function $\gamma'(x) \ge 0$ such that the argument maximising problem (11) solves the constrained problem (15).

PROOF. With the notation above, we have seen that u_n is increasing, v_n is decreasing, and $v_{n-1} - v_n$ is decreasing. Furthermore, by hypothesis $u_n - u_{n-1}$ is increasing, which by definition of v'_n means that $v'_{n-1} - v'_n$ is decreasing. In the following, we reason on v_n but the argument is identical if v_n is replaced by v'_n .

Let us fix x > 0. The constrained problem is

$$\min_{n} v_n \quad \text{ subject to } u_n <= x$$

while the maximum utility problem can be rewritten as

$$\min_{n} \left(v_n + \frac{1}{\gamma} u_n \right).$$

Since u_n is increasing, there is a highest $n_0 = n(x)$ such that some configuration satisfies the constraint, i.e. such that $u_{n_0} \le x$. Since v_n is decreasing, the solution of the constrained problem is found for $n = n_0$, for any configuration satisfying the constraint. We want to choose γ such that the solution of the maximum utility problem is also at n_0 , for a configuration satisfying the constraint. We show that we can choose γ such that taking $n \neq n_0$ leads to a larger value of $v_n + \frac{1}{2}u_n$.

From our hypotheses, we see that the ratio of $u_{n+1} - u_n$ and $v_{n+1} - v_n$ is increasing. For $n \leq n_0$, we will have

$$v_n + \frac{1}{\gamma} u_n \geqslant v_{n_0} + \frac{1}{\gamma} u_{n_0}$$

if we take

(61)
$$\gamma \geqslant \frac{u_{n_0} - u_{n_0 - 1}}{v_{n_0 - 1} - v_{n_0}}.$$

Note that if $v_{n_0} - v_{n_0+1} = 0$, since $v_n - v_{n+1}$ is decreasing it means that for $n \ge n_0$ we have also $v_n - v_{n+1} = 0$, and we can always restrict the reasoning to n_{max} being the highest nsuch that $v_n - v_{n+1} \neq 0$. For $n > n_0$, we will have

$$v_n + \frac{1}{\gamma} u_n \geqslant v_{n_0} + \frac{1}{\gamma} u_{n_0}$$

if

$$\gamma \leqslant \frac{u_{n_0+1} - u_{n_0}}{v_{n_0} - v_{n_0+1}}.$$

These two conditions can be satisfied since

$$\frac{u_{n_0} - u_{n_0 - 1}}{v_{n_0 - 1} - v_{n_0}} \leqslant \frac{u_{n_0 + 1} - u_{n_0}}{v_{n_0} - v_{n_0 + 1}}.$$

Choosing γ between those two bounds gives it as an increasing function of n_0 , thus as an increasing function of x.

As long as the sequence $(u_{n+1}^y - u_n^y)_{n=0...n_{\text{max}}}$ is increasing, maximising the utility and the constrained problem have the same solutions. This is not guaranteed in the general case, but can be ensured under the following condition.

LEMMA E.3. If $\forall n > 0$, $\exists i_0$, $\forall j = 1..n - 1$, $\Theta_{i_0}^{n+1} \cap \Theta_j^{n-1} = \emptyset$, the sequence $(u_{n+1} - u_n)_{n=1..n_{max}}$ is increasing.

PROOF. Let us suppose that $\exists n \geqslant 1$ such that $u_{n+1} - u_n < u_n - u_{n-1}$. Replacing by the explicit expression of u_n , the inequality is equivalent to

(62)
$$\sum_{i=1}^{n} I_{\Theta_i^n} - \sum_{i=1}^{n+1} I_{\Theta_i^{n+1}} < \sum_{i=1}^{n-1} I_{\Theta_i^{n-1}} - \sum_{i=1}^{n} I_{\Theta_i^n}$$

By hypothesis, $\exists i_0, \forall j = 1...n-1, \Theta_{i_0} \cap \Theta_j^{n-1} = \emptyset$, Eq. (62) can be written

(63)
$$\sum_{i=1}^{n} I_{\Theta_{i}^{n}} - \sum_{i=1, i \neq i_{0}}^{n+1} I_{\Theta_{i}^{n+1}} < I_{\Theta_{i_{0}}^{n+1}} + \sum_{i=1}^{n-1} I_{\Theta_{i}^{n-1}} - \sum_{i=1}^{n} I_{\Theta_{i}^{n}}$$

The term $I_{\Theta_{i_0}^{n+1}} + \sum_{i=1}^{n-1} I_{\Theta_i^{n-1}}$ is a sum of n I_{Θ_i} with disjoint Θ_i . By definition of Θ_i^n , the right hand side of the inequality is less than or equal to 0 and the left hand side of the inequality is greater than or equal to 0, which is absurd.

If
$$\forall i=1...n+1, \ \exists j=1...n-1, \ \Theta_i^{n+1}\cap\Theta_j^{n-1}\neq\emptyset$$
. In that case, we also have $\forall i, \ \exists j\in [\![1,n]\!] \ \Theta_i^n\cap\Theta_j^{n-1}\neq\emptyset$, otherwise due to lemma 3.2 this would lead to a contradiction. \square

If the condition of Lemma E.3 is not satisfied one can find a counter example where $u_{n+1}^y - u_n^y < u_n^y - u_{n-1}^y$ and the equivalence of utility maximisation and optimisation with constraints is not guaranteed. Finally, we have the desired result.

THEOREM E.4. Let us consider a dataset y and suppose that it verifies pattern separability at all orders, $n=1...n_{\max}$ then there exists an increasing function $\gamma(x)>0$ such that (10) and (14) have the same solution, and a function $\gamma'(x)>0$ such that (11) and (15) have the same solution.

PROOF. Under the hypothesis of separability, by lemma E.3, $(u_{n+1}^y - u_n^y)_{n=1...n_{\text{max}}}$ is increasing, and by lemma E.2, we have the desired result.

APPENDIX F: DATA ANALYSIS METHODS

In Section 5.3, we compare the performances of several methods, which we here describe in detail. We first make explicit a few terms. The Bayes factor (BF) here refers to the ratio $p(y \mid k+1)/p(y \mid k)$, where $p(y \mid k)$ is the Bayesian evidence defined in Eq. (6). We define the posterior number of planets (PNP) as

(64)
$$p(k \mid y) = \frac{p(y \mid k)p(k)}{\sum_{i=1}^{n_{\text{max}}} p(y \mid i)p(i)}$$

Furthermore, we here define the periodogram as in Delisle, Hara and Ségransan (2020a). This one is defined as a difference of log likelihoods of two models: a null hypothesis H_0 and a model K_{ω} with a sinusoidal component at frequency ω . The periodogram at frequency ω is defined as

(65)
$$\mathcal{P}(\omega) = \max_{\theta_{K_{\omega}}} \log p(y \mid \theta_{K_{\omega}}) - \max_{\theta_{H_0}} \log p(y \mid \theta_{H_0}).$$

Denoting by $\mathcal{N}(x, \mathbf{V})$ a multivariate Gaussian distribution of mean x and covariance \mathbf{V}

(66)
$$H_0: y \sim \mathcal{N}(0, \mathbf{V_0})$$

(67)
$$K_{\omega}: y = A\cos\omega t + B\sin\omega t + \epsilon, \ \epsilon \sim \mathcal{N}(0, \mathbf{V_0})$$

where V_0 is the covariance matrix used to generate the noise in our simulated datasets. The periodogram is computed on a tightly spaced grid of frequencies between frequency frequency ω_{\min} and ω_{\max} . Denoting by P^{\star} the maximum value of the periodogram, the false alarm probability (FAP) is defined as the probability that, knowing the null hypothesis, the maximum of the periodogram exceeds P^* . Denoting by Ω the grid of frequencies onto which the periodogram is computed,

(68)
$$FAP = p(\max_{\omega \in \Omega} \mathcal{P}(\omega) \geqslant \mathcal{P}^* \mid H_0)$$

We further use a ℓ_1 periodogram as defined in Hara et al. (2017). This algorithm searches for a representation of the data in the Fourier domain, penalizing the sum of their amplitudes with a ℓ_1 norm, thus enhancing the sparsity of the representation.

- Periodogram + FAP: The periodogram is computed with the same grid of frequencies as the one used to generate the data (from 1.5 to 100 d) and the correct covariance matrix. If the FAP is below a certain threshold fixed in advance, we add a cosine and sine function at the period of the maximum peak to the linear base model and recompute the periodogram. The planet is added if the FAP is below the FAP threshold. We do not search for a third
- Periodogram + Bayes factor: same as above, but here the criterion to add a planet is that the Bayes factor is above a certain threshold. The evidences (Eq. (6)) are computed with the distributions used in the simulations, in particular the period is left free between 1.5 and 100 days.
- ℓ_1 -periodogram³ + FAP: we compute the ℓ_1 periodogram (Hara et al., 2017) with the same grid of frequencies as the one used to generate the data (from 1.5 to 100 d). If the FAP of the maximum peak is below a certain threshold, it is added to the base model of unpenalized vectors, the ℓ_1 periodogram is recomputed, the FAP of the maximum peak is assessed. If it is below a certain threshold, the a planet detection is claimed. We do not look for a third planet.
- ℓ_1 -periodogram + Bayes factor: same as above, but here the criterion to add a planet is that the Bayes factor comparing n+1 versus n planet models is above a certain threshold.
- FIP: We compute the FIP periodogram as defined in section 2.3 and select the two highest peaks. We select a period if its corresponding FIP is below a certain threshold.
- PNP + FIP periodogram: here, to select the number of planets we order the peaks of the FIP periodogram with increasing FIP. We select the number of peaks corresponding to the highest posterior number of planets as defined in Eq. (64).
- FIP periodogram + Bayes factor: the periods are selected as the highest peaks of the FIP periodogram and the number of planets is selected with the Bayes factor. This procedure is very close to Gregory (2007) except that we use the FIP periodogram instead of the marginal distribution of periods for each planets. We do not take the approach of Gregory (2007) to select the periods as nested sampling algorithms such as POLYCHORD tend to swap the periods of planets, such that marginal distributions are typically multi-modal.
- FIP periodogram + FAP: the periods are selected as the highest peaks of the FIP periodogram and the number of planets is selected with the false alarm probability.

 $^{^3}$ The ℓ_1 periodogram code is available at https://github.com/nathanchara/l1periodogram