ABSTRACT

In a Bayesian context, theoretical parameters are correlated random variables. Then, the constraints on one parameter can be improved by either measuring this parameter more precisely - or by measuring the other parameters more precisely. Especially in the case of many parameters, a lengthy process of guesswork is then needed to determine the most efficient way to improve one parameter’s constraints. In this short article, we highlight an extremely simple analytical expression that replaces the guesswork and that facilitates a deeper understanding of optimization with interdependent parameters.

Key words: cosmic background radiation – cosmological parameters – methods: analytical – methods: data analysis

1 INTRODUCTION

The Fisher matrix has become widely spread in cosmology since it allows quick forecasts of parameter constraints in the limit of a Gaussian posterior likelihood. Recent works on the Fisher matrix extend the formalism also to errors in the independent variables (Heavens et al. 2014) and to non-Gaussianity (Sellentin et al. 2014; Sellentin 2015; Joachimi & Taylor 2011). Its ease of handling can be traced back to many analytical operations that can be performed on a multivariate Gaussian and that can be summarized in a manual-like collection:

- in order to maximize a parameter, i.e. fixing it to its bestfit value, the rows and columns of this parameter must be removed from the Fisher matrix
- the removal of rows and columns from the inverse of the Fisher matrix leads to a marginalization of the respective parameter
- a combination of independent experiments with the same fiducial or best fit can be achieved by adding up their Fisher matrices
- a transformation of variables can be achieved by multiplying the Fisher matrix on the left and the right with the Jacobian matrix of the transformation and its transpose.

To this Fisher matrix manual, we now want to add a further rule that allows optimizing an experiment, answering the question: Given \( n \) correlated parameters \( \theta_1,...,\theta_n \), and not being able to improve the measurement of the parameter \( \theta_i \), which other parameter \( \theta_k \) should we measure more precisely in order to best improve the constraints on \( \theta_i \), and which gain in the precision of \( \theta_i \) can then be expected? For clarity, in the following we refer to the \( i \)-th parameter as the target parameter and to the \( k \)-th parameter as the control parameter which shall emphasise that we expect to better control the accuracy of this parameter with future experiments.

This problem can occur in a variety of situations. Let us take a typical case in cosmological applications. In a standard analysis of CMB data (see e.g. Planck Collaboration et al. (2014a)), one has parameters that depend on early cosmology (e.g. the spectral index \( n_s \)), parameters that depend on the local late-time universe, e.g. the Hubble constant \( H_0 \), and parameters that depend on totally different physics, e.g. the “nuisance” parameters that describe some foreground contamination, e.g. the amplitude of the cosmic infrared background \( A_{\text{cib}} \).

The usual way to answer this question is to invert the parameter covariance matrix (which is normally what the experiment
Figure 1. Correlation matrix of the Planck cosmology and nuisance parameters. The first 6 columns and rows are the cosmological parameters $\omega_b, \omega_cdm, H_0, A_s, n_s, \tau_{reio}$ which are strongly correlated amongst each other. The remaining columns are the nuisance parameters $A^{ps}_{100}, A^{ps}_{143}, A^{ps}_{217}, A^{cib}_{143}, A^{cib}_{217}, A_{ksz}, \rho_{ps}, \rho_{cib}, n_{Dl_{cib}}, D^{cal}_{100}, D^{cal}_{217}, \xi_{cib}/A_{ksz}, B_{m1,1}$ whose meanings are explained in (Planck Collaboration et al. 2014b). The marked column contains the correlations of $n_s$.

provides) deriving a Fisher matrix, add priors to the Fisher matrix that shall quantify the expected future gain in measurement precision of the control parameters, and invert again. The updated covariance of the target parameter will then be a diagonal element of this inverse matrix. If the prior is found to produce a strong decrease in the variance of the target parameter, one would typically undertake even big scientific efforts in order to really establish a measurement that can produce such a constraint as the prior. On the other hand, if the target parameter does not react sensitively to an improvement in the constraint of the control parameter, one would not need to measure the control parameter better.

Searching for effective priors by adding them to a Fisher matrix and inverting is per se a simple operation, but repeating it for any pair of target/control parameters and for any possible value of the prior will rapidly become a tedious and lengthy process if the covariance matrix contains dozens of parameters. Additionally repetitive inversions are prone to numerical uncertainties. The complexity of possible combinations of target/control parameters further increases if a correlated set of control parameters shall be improved upon with priors. The rest of this short note is devoted to deriving and discussing an analytical formula that drastically simplifies the procedure.

At the time of the first version on this archive, we wrote that "To the best of our knowledge, this simple formula seems not to have been pointed out before". After publishing this paper, however, Eric Linder made us notice that the formula has actually been derived earlier in Astier (2001).

2 THE SHERMAN-MORRISON-WOODBURY FORMULA

The idea is entirely based on the Sherman-Morrison-Woodbury formula (Sherman & Morrison 1950; Woodbury 1950). This formula states that if $M$ is a square matrix and $u, v$ are vectors then

$$(M + uv^T)^{-1} = M^{-1} - M^{-1}uv^TM^{-1} \frac{1}{1 + v^TM^{-1}u}$$

(1)

where $T$ denotes transposition. The formula allows to quickly find the inverse of $M$ when a matrix $uv^T$ is added to $M$. If we demand that $M$ is a non-degenerate Fisher matrix, i.e. the inverse of the covariance matrix of parameters, then $M$ is symmetric and positive definite. If we further set $u = v$, we can construct a prior matrix $P = uu^T$ where the vector $u$ is

$$u = \{0, 0, \ldots p^{-1}_k, \ldots\} = p^{-1}_k \hat{u}$$

(2)

where $p_k$ is the prior standard deviation on the control parameter $\theta_k$, that shall quantify the expected improvement on $\theta_k$ in a feasible future experiment. The vector $\hat{u}$ is the $k$-th basis vector. Introducing a matrix $\hat{P} = \hat{u}\hat{u}^T$ i.e. a matrix whose elements are all zero except for $\hat{P}_{kk} = 1$, we can write $P = p_k^2\hat{P}$, and Eq. (1) then specializes to

$$(M + P)^{-1} = M^{-1} - \frac{M^{-1}PM^{-1}}{1 + \text{Tr}(PM^{-1})}.$$
A new tool for Fisher matrix forecasts

The variance $\sigma_i^2$ of our target parameter $\theta_i$, after having marginalized over all other parameters, is given by $\sigma_i^2 = M^{-1}_{ii}$. Its improved variance $\sigma_{i,\text{new}}^2$ after having added a prior to the $k$-th control parameter is then

$$\sigma_{i,\text{new}}^2 = (M + P)^{-1}_{ii}$$

$$= M^{-1}_{ii} - \frac{(M^{-1}PM^{-1})_{ii}}{1 + \text{Tr}(PM^{-1})}$$

$$= M^{-1}_{ii} - \frac{P_k^{-2}(M^{-1}PM^{-1})_{ii}}{1 + p_k^{-2}\text{Tr}(PM^{-1})}$$

$$= \sigma_i^2 - \frac{p_k^{-2}(M^{-1}PM^{-1})_{ii}}{1 + p_k^{-2}\sigma_k^2}$$

Now we use the fact that the fully marginalized variance of the control parameter is $\text{Tr}(\hat{P}M^{-1}) = \sigma_k^2$ and

$$(M^{-1}\hat{P}M^{-1})_{ii} = \rho_{ik}^2\sigma_i^2\sigma_k^2$$

where $\rho_{ik} = M^{-1}_{ii} \sqrt{M^{-1}_{kk}}$ is the correlation coefficient and one has $|\rho_{ik}| \leq 1$ because of positive-definiteness of $M$. So we derive our main result

$$\sigma_{i,\text{new}}^2 = \sigma_i^2 - \frac{\rho_{ik}^2\sigma_i^2\sigma_k^2}{p_k^{-2} + \sigma_k^2}$$

which describes directly and transparently how the variance of the target parameter $\theta_i$ decreases if we measure better the parameter $\theta_k$.

Also, if the prior on the control parameter $k$ is very weak, i.e. $p_k \to \infty$, the error $\sigma_i$ of the target parameter, does not change. This equation can be trivially applied even when the control parameter coincides with the target parameter, by putting $i = k$ and the self correlation $\rho_{ik} = 1$.

From the previous equation, the decrease $\Delta\sigma_i^2 = \sigma_{i,\text{new}}^2 - \sigma_i^2$ follows to be

$$\frac{\Delta\sigma_i^2}{\sigma_i^2} = -\frac{\rho_{ik}^2}{1 + \varepsilon}$$

where $\varepsilon = p_k^{-2}/\sigma_k^2$. This tells us that if we add a prior to the error on the control parameter which is $\varepsilon$ times the current error, then the target parameter constraint decreases by a fraction $\rho_{ik}^2/(1 + \varepsilon)$. At most, the fractional decrease is then $\rho_{ik}^2 \leq 1$. So the very simple recipe for choosing the most convenient control parameter to improve the estimation of the target parameter, is to select the most correlated one. This of course was to be entirely expected; our formula (11) quantifies the effect in a very simple way as a function of the correlation coefficient and of the ratio $\varepsilon$.

A generalization to several control or target parameters is described in the Appendix.
3 EXAMPLE: INDIRECTLY IMPROVING CMB CONSTRAINTS ON THE PRIMORDIAL SLOPE

For a mere illustrative purpose, we consider now the actual parameter covariance matrix $C$ for Planck (Planck Collaboration et al. 2014a) as published in the package Monte Python (Audren et al. 2013) and assume that the posterior is well approximated by a multivariate Gaussian, such that we can interpret $C$ as an inverse Fisher matrix.

Since Planck does not take any data anymore, it will not improve directly the measurement of any cosmological parameters. It is however well known that Planck has many nuisance parameters that are degenerate with the primary cosmological parameters (Planck Collaboration et al. 2014b). Therefore, the constraining power of the Planck data set can be boosted by constraining these nuisance parameters better, but how much gain can be expected from this, and which nuisance parameter should be tackled with the most effort? For example, the amplitude of the cosmic infrared background (CIB) is a nuisance parameter for Planck, and can in principle be constrained with new observations independent of Planck. The same goes for other cosmological parameters, e.g. the Hubble constant $H_0$.

Let’s assume we want to constrain the spectral index $n_s$ more precisely because we are interested in inflationary physics, i.e. $n_s$ is our target parameter. With the formalism developed in the previous section, we can now search for the most effective control parameter to achieve this: We use the Planck baseline covariance matrix $C$ and dissect it into a correlation matrix $R$

$$R_{ij} = \frac{C_{ij}}{\sqrt{C_{ii}C_{jj}}}$$

(12)

The resulting correlation matrix is depicted in Fig. (1). From the fifth column we see that $n_s$ is most correlated with the Hubble constant $H_0$ with a correlation coefficient of $p_{n_s, H_0} = 0.81$. So constraining $n_s$ indirectly can best be achieved by better constraining the Hubble constant $H_0$ through local measurements, see e.g. Riess et al. (2011).

Second best choice would be constraining $\omega_{cdm}$ ($p_{n_s, \omega_{cdm}} = -0.8$), third best would be constraining $\omega_b$, due to $p_{n_s, \omega_b} = 0.56$. Next follows the optical depth $\tau_{ee,io}$ with $p_{n_s, \tau_{ee,io}}=0.4$ which can be independently constrained through radio observations of the dark ages. The best choices for improving upon nuisance parameters are the parameters that specify Planck’s phenomenological model of the cosmic infrared background. Planck uses a power-law model for the CIB-spectrum, whose amplitudes in the different Planck channels are parameterized by the nuisance parameters $A_{217}^\text{cib}$, $A_{81}^\text{cib}$ and the correlation between the two channels is given by the nuisance parameter $p_{\tau_{ee,io}}^{217\times81}$. The kinetic Sunyaev-Zeldovich effect also possesses a relatively high correlation with $n_s$. All of these nuisance parameters are correlated with $n_s$ on the order of 0.1 so that we can expect at most an improvement of 1% on $n_s$ for each perfectly measured nuisance parameter.

In Fig. (2), employing Eq. (10), we plot by how much the constraints on $n_s$ reduce, given an improved estimate of any of the named parameters. For instance, an independent prior on $H_0$ that is as good as the current Planck uncertainty (i.e. $\varepsilon = 1$) will decrease the variance of $n_s$ by $0.81^2/2 = 0.325$ times the old variance, i.e. $\sigma_{n_s}$ will improve by 18%. At most, the error on $n_s$ can improve by 41% by a perfect determination of $H_0$. By applying the Eq. (23) in Appendix, we obtain a reduction of the standard deviation from the current Planck value $\sigma_{n_s} = 0.0073$ down to $\sigma_{n_s} = 0.0063$ if all the nuisance parameters were precisely known and $\sigma_{n_s} = 0.0025$ if all the parameters, except obviously $n_s$ itself, were precisely known.

4 CONCLUSIONS

The Sherman-Morrison-Woodbury formula allows to calculate the inverse of a perturbed matrix. We have described its application to a covariance matrix or a Fisher matrix, whose inverse is of particular interest since its diagonal elements represent the fully marginalized errors on parameters. We used priors in order to parameterize the gain by potential future experiments or theoretical efforts, that would only be undertaken if they effectively break degeneracies and thereby lead to big improvements in the fully marginalized errors.

Under the addition of priors to the Fisher matrix, the marginalized errors of course decrease. However, the magnitude of the decrease could not be foreseen in a transparent way by the standard procedure of inverting the Fisher matrix. The Sherman-Morrison-Woodbury formula instead provides an analytical result that allows to judge quickly how the addition of priors on one parameter, will propagate through to the constraints on other parameters.

The conclusion of this paper is summarized in a new bullet point to the manual of the Fisher matrix:

- When a prior $p_{\theta_i}$ on parameter $\theta_i$ is added, then the variance of the parameter $\theta_i$ will decrease as prescribed by Eq. (10).

This new rule provides an effective guidance to where modern cosmology should put the most effort, in order to quickly break parameter degeneracies and improve the constraints of interdependent parameters. For an exactly (approximately) Gaussian posterior likelihood, this result holds exactly (approximately). If the posterior is moderately non-Gaussian, the covariance matrix (as estimated from an MCMC run) and the Fisher matrix, tend to not agree anymore. Applying the here presented tool to the MCMC-covariance matrix might then still provide a good guidance, although it should not be applied to the Fisher matrix. If however, there exists additionally a strongly pronounced genuine $n$-point function for $n > 2$, then analytical
marginalizations are not possible anymore, and the analytical tool here presented is no longer well suited. Then, refuse to numerical brute force must be sought.

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APPENDIX: GENERALIZATION TO SEVERAL PARAMETERS

Eq. (10) can be generalized to several control parameters but the explicit formulae for the general case become rapidly very cumbersome. Any symmetric prior matrix $P$ acting on $N$ control parameters (i.e. containing non-zero entries only for a subset of $N$ rows and columns) can be written as

$$P = \sum_{k=1}^{N} \lambda_k u_k u_k^T \equiv \sum_{k=1}^{N} P_k$$

(13)

where $\lambda_k$ are the eigenvalues of $P$ and $u_k$ is the $k$-th orthonormal eigenvector. Then the new Fisher matrix becomes $M+\sum P_k$ where every $P_k$ is in the form required for Eq. (1) and repeated application of the Sherman–Morrison–Woodbury formula generates the result. For just two control parameters, $\theta_n$ and $\theta_k$, the final result will depend on the three independent entries of the symmetric submatrix $M_{nk}$, the three independent entries of the prior matrix that add information on $\theta_n$ and $\theta_k$, the two correlation coefficients $\rho_{nk,\rho_{kk}}$, and on the initial variance $\sigma_i^2$, so a total of 9 quantities. For $N$ control parameters the formula depends on $(N+1)^3$ quantities.

A prior matrix $P$ that adds information on the two control parameters $\theta_n$ and $\theta_k$ will only have three distinct non-zero elements $P_{nk}, P_{nn}$ and $P_{kk}$. It can be decomposed as

$$P = \lambda_1 u_1 u_1^T + \lambda_2 u_2 u_2^T$$

(14)

where, $u_1 = (\cos \phi, -\sin \phi)$ and $u_2 = (\sin \phi, \cos \phi)$. In term of the elements of $P$ we have

$$\sin(2\phi) = \frac{2P_{kn}}{Q}$$

$$\cos(2\phi) = \frac{P_{nn} - P_{kk}}{Q}$$

(15) (16)

where $Q = \sqrt{(P_{kk} - P_{nn})^2 + 4P_{kn}^2}$ and similarly

$$\lambda_\pm = (P_{nn} + P_{kk} \pm Q)/2$$

(17)

We can then quote the final result that generalizes Eq. (10) to two control parameters $\theta_n, \theta_k$:

$$\sigma_{i,new}^2 = \sigma_i^2 \left[ 1 - \frac{S(\rho_{nk}^2, \sigma_n^2, \sigma_k^2) + 2\rho_{nk}\sigma_n\sigma_k \cos(2\phi) - D \lambda_+ \lambda_-}{2\Delta_{nk}\lambda_+ \lambda_- + S(\sigma_n^2 + \sigma_k^2) + D(\sigma_n^2 - \sigma_k^2) \cos(2\phi) - 2D\rho_{nk}\sigma_n\sigma_k \sin(2\phi) + 2} \right]$$

(18)

where

$$\Pi = \rho_{nk}^2 - 2\rho_{nk}\rho_{nn}\rho_{kk} + \rho_{nk}^2$$

(19)

$$S = \lambda_+ - \lambda_-$$

(20)

$$D = \lambda_+ \lambda_-$$

(21)

and $\Delta_{nk} = (1 - \rho_{nk}^2)\sigma_n^2\sigma_k^2$ is the determinant of the $nk$-submatrix. If $\rho_{nk} = \rho_{nn} = \phi = 0$ and $\lambda_- = \rho_{kk}^{-2}$, we are back to the 1-parameter case. In the limit of an infinitely strong prior (i.e. knowing the control parameters precisely) one gets the best possible estimation of the target parameter $\theta_i$.

$$\sigma_{i,new}^2 = \sigma_i^2 \left[ 1 - \frac{\rho_{nk}^2 + \rho_{kk}^2 - 2\rho_{nk}\rho_{kk}}{1 - \rho_{nk}^2} \right] = \sigma_i^2 \frac{\det R^{ikn}}{\det R^{nn}}$$

(22)

where $R^{nn}$ is the correlation matrix of the three parameters $\theta_i, \theta_k, \theta_n$, where we use upper indices to avoid confusion with matrix elements which are denoted with downstairs indices. $R^{nn}$ is obtained as in Eq. (12) i.e. by taking only the $i, k, n$ rows and columns of $M^{-1}$ and dividing each entry on the $a$th row and $b$th column by $\sigma_a\sigma_b$. Similarly, $R^{nk}$ is the correlation matrix of the parameters $\theta_k$ and $\theta_n$. It can be shown that the quantity in square brackets lies always between zero and unity, as it should be since a prior adds information and the variance cannot increase.

The last expression Eq. (22) generalizes to a set of arbitrary many precisely known control parameters in the form

$$\sigma_{i,new}^2 = \sigma_i^2 \frac{\det R^{iC}}{\det R^C}$$

(23)
where $\mathcal{C} = \{kmn...\}$ represents the set of an arbitrary number of control parameters. Eq. (23) can be proven as follows.

A well-known generalization of Cramer’s rule for inverting matrices is

$$\det(A^{-1})' = \frac{\det(A)'}{\det A}$$  \hspace{1cm} (24)

where $A$ is a $n \times n$ matrix, $\det A'$ is the determinant of the submatrix obtained by keeping only the rows and columns of the subset $J$, and $J'$ is the complementary subset, such that every index appears either in $J$ or in $J'$.

Now, since a correlation matrix is connected to the covariance matrix via

$$R = \text{diag}(1/\sigma_1, ..., 1/\sigma_n) \mathcal{C} \text{diag}(1/\sigma_1, ..., 1/\sigma_n)$$  \hspace{1cm} (25)

where $\text{diag}(1/\sigma_1, ..., 1/\sigma_n)$ is the diagonal matrix of the standard deviations, Eq. (23) can be written as

$$\sigma^2_{i,\text{new}} = \frac{\det \mathcal{C}_{i,\mathcal{C}}}{\det \mathcal{C}}$$  \hspace{1cm} (26)

We also know that $\sigma^2_{i,\text{new}}$ is obtained by maximizing the control parameters, i.e. by inverting the covariance matrix $\mathcal{C}$, striking out the rows/columns corresponding to the $\mathcal{C}$ subset so to produce the matrix $(\mathcal{C}^{-1})'^{\mathcal{C}'}$, where $\mathcal{C}'$ is the complementary set of parameters to $\mathcal{C}$. This matrix then needs to be inverted again and the entry $\mathcal{C}_{ii}$ is then $\sigma^2_{i,\text{new}}$.

This entry will however be given by the minor determinant of the $i$-th element of $(\mathcal{C}^{-1})'^{\mathcal{C}'}$ divided by the determinant of $(\mathcal{C}^{-1})'^{\mathcal{C}'}$. That is, using in the last step Eq. (24),

$$\sigma^2_{i,\text{new}} = \frac{\det((\mathcal{C}^{-1})'^{\mathcal{C}'})}{\det(\mathcal{C})} = \frac{\det \mathcal{C}_{i,\mathcal{C}}}{\det \mathcal{C}}$$  \hspace{1cm} (27)

where the notation $(i, \mathcal{C}')$ means the index subset formed by all the indexes except the $i$-th one and the $\mathcal{C}$ subset.

Eq. (23) then gives a handy expression to determine the best possible estimate of the target parameter in the limit of an exact determination of the control parameters. Most experiments provide directly the parameter covariance or correlation matrix, obtained for instance through a Monte Carlo Markov Chain procedure; our expression can be immediately applied to the correlation matrix and no matrix inversion is needed.

Finally, we quote for completeness a further generalization to any number of target parameters but valid only when all the other parameters are considered control parameters, and again in the limit of an infinitely strong prior. This relation is well known in statistics because it gives the conditional covariance, i.e. the covariance when some of the random variables are known. Denoting with $\mathcal{T}$ the set of target parameters, we have

$$\det \mathcal{C}_{\mathcal{C}^{\text{new}}}(\mathcal{T}) = \frac{\det \mathcal{C}_{\mathcal{C}^{\text{new}}}(\mathcal{T},\mathcal{C'})}{\det \mathcal{C}}$$  \hspace{1cm} (28)

The inverse of the determinant of the submatrix $\mathcal{C}^{\mathcal{T}}$ is often called a figure-of-merit. So this expression tells us how much the figure-of-merit improves when all the other parameters are fixed, i.e. the best possible figure-of-merit one can achieve by improving the constraints on correlated parameters.

REFERENCES

Astier P., 2001, Phys. Lett., B500, 8
Audren B., Lesgourgues J., Benabed K., Prunet S., 2013, JCAP, 2, 1
Heavens A. F., Seikel M., Nord B. D., Aich M., Bouffanais Y., Bassett B. A., Hobson M. P., 2014, MNRAS, 445, 1687
Joachimi B., Taylor A. N., 2011, MNRAS, 416, 1010
Planck Collaboration Ade P. A. R., Aghanim N., Armitage-Caplan C., Arnaud M., Ashdown M., Atrio-Barandela F., Aumont J., Baccigalupi C., Banday A. J., et al. 2014a, A. & A., 571, A15
Planck Collaboration Ade P. A. R., Aghanim N., Armitage-Caplan C., Arnaud M., Ashdown M., Atrio-Barandela F., Aumont J., Baccigalupi C., Banday A. J., et al. 2014b, A. & A., 571, A16
Riess A. G., Macri L., Casertano S., Lampeitl H., Ferguson H. C., Filippenko A. V., Jha S. W., Li W., Chornock R., 2011, APJ, 730, 119
Sellentin E., 2015, MNRAS, 453, 893
Sellentin E., Quartin M., Amendola L., 2014, MNRAS, 441, 1831
Sherman J., Morrison W. J., 1950, Ann. Math. Statist., 21, 124
Woodbury M., 1950, Statistical Research Group, Memo Rep. No. 42

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