The development of a space climatology: 3. Models of the evolution of distributions of space weather variables with timescale

Article


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Introduction

Part 1

This supporting information gives details of the Maximum Likelihood Estimation (MLE) method and associated goodness-of-fit metrics

Part 2

The values of best-fit parameters (and their uncertainties) and the goodness-of-fit metrics are presented for the fits of 7 selected distribution forms to the observed distributions of the geomagnetic indices, \(a_p\) and \(Dst\) and the estimated power into the magnetosphere, \(P_\alpha\) (all expressed as ratios of
their annual means). The procedures are repeated for data averaged over timescales \( \tau \) of 3 hours, 1 day, 7 days, 27 days, 0.5 years and 1 year. Plots of the observed and fitted distributions (both probability density functions (p.d.f.s) and cumulative distribution functions (c.d.f.s) are also presented for all cases.

**Part 3**

A Table giving a list in rank order of the 83 largest storms (the top 0.25%) defined by daily mean \( Ap \)

**Part 1. Maximum Likelihood (MLE) method and associated goodness-of-fit metrics**

Probability density distributions can be fitted to data using the least squares method. This involves counting the fraction of all samples in bins, \( P_o \), of arbitrarily-chosen width to create a histogram and then evaluating the adopted pdf function for the bin centers, \( P_m \). The mean square of the deviation is then computed, \( \Delta = \langle (P_m - P_o)^2 \rangle \) and the parameters describing the fitted distribution iterated until the minimum \( \Delta \), \( \Delta_{MS} \), is obtained. One major problem with this “least squares” fit is that the results can depend on the bin width chosen [e.g., Woody et al., 2016] and it assumes that the fit residuals are normally distributed.

Maximum Likelihood Estimation (MLE) provides an alternative that avoids these problems. It is a generalization of the least squares method, which it reduces to if all the assumptions of least squares are met. MLE searches for the parameter values of the distribution form used that maximize a likelihood function, given the observations. The likelihood is estimated from the joint probability of the assumed distribution generating the \( N \) observed data points \( x_1, x_2, ..., x_N \) for a parameter \( a \). (For simplicity we here consider a distribution with just one fit parameter, \( a \): in general there can be several). For independent measurements this is given by the product of the individual densities \( p(x|a) \), which is the likelihood

\[
L(a) = p(x_1|a) \times p(x_2|a) \times ... \times p(x_i|a) \times ... \times p(x_N|a) = \prod_{i=1}^{N} p(x_i|a)
\]

For a number of reasons is easier to work with natural logarithm of \( L \), the log-likelihood \( F(a) \)

\[
F(a) = \log_n(L) = \sum_{i=1}^{N} \log_n(p(x_i|a))
\]

MLE finds the parameter value \( a \) that maximizes \( L(a) \), the maximum likelihood being \( L_m \)

There are two goodness-of-fit metrics that can be used in MLE. The \( AIC \) is the Akaike Information Criterion metric and the \( BIC \) the Bayesian (or Schwarz) Information Criterion. Where

\[
AIC = 2d_f - 2\log_n(L_m)
\]

where \( d_f \) is the number of fit parameters (degrees of freedom) and
\[ BIC = \log_n(N) \times d_i - 2\log_n(L_m) \]

The AIC and BIC values are not (unlike \( \Delta MS \)) absolute quality metrics because they depend on the data sample set of \( x \) values in question. However, they can be used to compare the goodness-of-fit of different distributions to the same set of \( x \) data, the smallest value indicating the largest maximum likelihood \( L_m \). The first term means that the number of degrees of freedom of the fit are allowed for and the BIC in gives larger weight to this factor than the AIC provided the number of samples \( N \) exceeds 7. Hence AIC and BIC are useful in evaluation which distribution best fits the data.

One other goodness-of-fit test we apply is the modified Kolmogorov–Smirnov test which yields the metric \( D \) which is the largest absolute value of the difference of the observed and fitted cumulative distribution functions (c.d.f.s). These c.d.f.s can be evaluated without binning the data and the K-S test is a non-parametric test as it does not assume that the data are normally distributed.

**Part 2. Results of maximum likelihood (MLE) fitting to observed distributions of geomagnetic indices \( ap \) and \( Dst \) and of the power input into the magnetosphere, \( P_\alpha \)**

This section presents Tables giving best-fit parameters and their 2-\( \sigma \) uncertainty ranges and the goodness of fit metrics (and their rank orders) for 7 different standard distribution forms. The forms used are:

- normal (Gaussian) distribution
- lognormal distribution
- Weibull distribution
- Burr distribution
- Gamma distribution
- Log-logistic distribution
- Rician distribution

For all these distributions the number of degrees of freedom is \( d_i = 2 \), except the Burr for which \( d_i = 3 \). These distributions are fitted to the ratios of observed \( \langle ap \rangle / \langle ap \rangle_{1yr} \), \( \langle Dst \rangle / \langle Dst \rangle_{1yr} \) and \( \langle P_\alpha \rangle / \langle P_\alpha \rangle_{1yr} \) - in each case for 6 different values of averaging timescale \( \tau \), namely: 3hrs (the basic resolution of the \( ap \) data), 1 day, 7 days, 27 days, 0.5 year and 1 year. In each case, a plot is given of both the observed and best-fit (MLE) cumulative distribution functions (c.d.f.s) and of the corresponding probability density functions (p.d.f.s). Note that in the case of the observed p.d.f.s, the data samples have been binned (to give a histogram) into 150 contiguous bins centered on \([0.5:1:150](x_{98}/100)\) where \( x_{98} \) is the 98th percentile of the observed distribution and the numbers of samples \( n \) in each bin then normalized so that \( \Sigma n(x_{98}/100) \) is unity.

For the distributions of \( \langle ap \rangle / \langle ap \rangle_{1yr} \), the lognormal distribution form consistently performs best in all four metrics until \( \tau \) gets large and the distribution becomes close to normal. Note that in these large-\( \tau \) cases, the AIC and BIC have both turned negative because the maximum likelihood, \( L_m \) exceeds unity. (It is often said that \( L_m \) cannot exceed unity but this is incorrect and this means that the log likelihood can be positive). However, this only happens when the fits are of extremely high quality (as seen in the plots). As all the tested distributions tend to Gaussians in one limit, all distributions fit the
high $\tau$ distributions very well and the rank orders are based on minimal differences in the metrics – i.e. the fitted distributions are essentially all equally valid. Note for $\tau = 1$ year the distribution of and parameter $<x>_/\tau$ $<x>_{1yr}$ is a delta function at unity which is a Gaussian of unity mean 1 and standard deviation zero.

The behavior is quite similar for the distributions of normalized power input to the magnetosphere $<P_{\alpha}>_/\tau$ $<P_{\alpha}>_{1yr}$ except at the lowest $\tau$ where the lognormal does not fit the observations well. For $\tau$ of 7 days and 27 days the lognormal is best by all metrics and, as for $ap$, at the larger $\tau$ all distributions fit the near-Gaussian form well and the lognormal is, effectively, as good as any other form. The distribution at $\tau = 3$ hours is complex in form and in Paper 2 is explained as the effect of averaging (via the central limit theorem) on the very non-standard distribution at $\tau = 1$ min in the IMF orientation factor. In Paper 2 it was described in terms of a Weibull distribution which fits the above-the-mode values very well but does not fit the mode and below quite as well as the Burr distribution (see Figures S13 and S14). Table S6 shows that both the AIC and BIC metrics indicate that the addition of an extra shape parameter in the Burr is valid in this case. The advantage gained in using the Burr is a better fitting of the near-zero peak but the fits to the distribution above the mode are very similar.

In contrast, for the distributions of $<Dst>_/\tau$ $<Dst>_{1yr}$ the lognormal distribution is never the best option. Of the two-parameter distribution fits the Gamma and the Weibull distributions are very similar in all their goodness of fit estimates and the best options for $\tau$ up to 0.5 year, above which all distributions fit the near-Gaussian observed distribution well. However, at 7 days and below the Burr distribution is best, even in the BIC metric that penalises the extra degree of freedom most. The Figures S7 to S11 show that the 2-parameter fits match the distribution above the mode well but have trouble matching the exact form of the peak around the mode.
Table S1. Best-fit parameters and their 2-σ uncertainty ranges for γ tested distribution forms fitted to the ratio $<\Delta p>/\sqrt{<\Delta p>^2}$ for the ap geomagnetic index data for 6 different values of $\tau$. The distributions studied are: the normal (Gaussian) distribution (for which the parameter $A$ is the mean, $m$; and parameter $B$ is the standard deviation, $\sigma$); the Lognormal distribution ($A = \mu$, the mean of logarithmic values; $B = \sigma$, the standard deviation of logarithmic values); the Weibull ($A = \lambda$, the scale parameter; and $B = k$, the shape parameter); the Burr distribution ($A = \lambda$, the scale parameter, $B = k$, the first shape parameter, and $C = k_2$, a second shape parameter); the Gamma distribution ($A = k$, the shape parameter, and $B = \lambda$, the scale parameter); the Log-logistic distribution ($A = m$, the mean; and $B = k$, the shape parameter); and the Rician distribution ($A = \sigma$, the noncentrality parameter and $B = \lambda$, the scale parameter). In each case the optimum fit is given, along with the minimum and maximum of the 2-σ uncertainty range, as derived using the Maximum Likelihood Estimation (MLE) method (using the MATLAB statistics toolbox). Fits are carried out using averaging intervals of $\tau$ of 3hrs (the basic resolution of the ap data), 1 day, 7 days, 27 days, half a year and 1 year.

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**Table S2.** Goodness-of-fit metrics for the 7 tested distribution forms and the \( ap \) geomagnetic index ratio \( <ap>-/<ap>_\text{r}_{\text{year}} \) data averaged over intervals of duration \( \tau \) described in Table S1. \( D \) is the largest absolute value of the difference of the observed and fitted cumulative distribution functions (c.d.f.s) obtained from a modified version of the non-parametric Kolmogorov–Smirnov test; \( \Delta_{MS} \) is the mean square deviation of the observed and fitted probability distribution functions (p.d.f.s) for 150 contiguous bins centered on \( <ap>-/<ap>_\text{r}_{\text{year}} = [0.5:1:150](X_{98}/100) \) where \( X_{98} \) is the 98th percentile of the observed \( <ap>-/<ap>_\text{r}_{\text{year}} \) distribution. \( N \) is the total number of available samples, \( \text{AIC} \) is the Akaike Information Criterion metric from the maximum likelihood estimate, and \( \text{BIC} \) the Bayesian Information Criterion. The last 4 columns give the rank order in goodness-of-fit for a given \( \tau \) according to these four metrics. Note all distributions have two degrees of freedom, except the Burr that has 3.

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Figure S1. Best-fit distributions (in colours) fitted using the MLE method to the observed distributions (in black) for 7 tested distribution forms fitted to that for the ratio $\frac{<ap>}{<ap>_{\tau=1yr}}$ of the $ap$ geomagnetic index data and an averaging timescale $\tau = 3$ hours. The plot on the right shows the probability distribution functions (pdfs) and on the left the corresponding cumulative distribution functions (cdfs). The fitted distributions are: (cyan) the normal (Gaussian) distribution; (mauve) the Lognormal distribution; (green) the Weibull distribution; (blue) the Burr distribution; (red) the Gamma distribution; (orange) the LogLogistic distribution; and (brown) the Rician distribution. The optimum distribution parameters are given in Table S1 and the goodness-of-fit metrics in Table S2.
Figure S2. Same as Figure S1 but for an averaging timescale $\tau = 1$ day.

Figure S3. Same as Figure S1 but for an averaging timescale $\tau = 7$ days.
Figure S4. Same as Figure S1 but for an averaging timescale $\tau = 27$ days.

Figure S5. Same as Figure S1 but for an averaging timescale $\tau = 0.5$ year.
Figure S6. Same as Figure S1 but for an averaging timescale $\tau = 1$ year.
Table S3. Same Table S1 for the ratio $<\text{Dst}>_{\tau}/<\text{Dst}>_{\tau_{\text{asyr}}}$ of the Dst geomagnetic index data

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**Figure S7.** Same as Figure S1 but for the ratio $\frac{<\text{Dst}>}{<\text{Dst}>}$ of the ap geomagnetic index data (and for an averaging timescale $\tau = 3$ hours).

**Figure S8.** Same as Figure S7 but for an averaging timescale $\tau = 1$ day.
Figure S9. Same as Figure S7 but for an averaging timescale $\tau = 7$ days.

Figure S10. Same as Figure S7 but for an averaging timescale $\tau = 27$ days.
Figure S11. Same as Figure S7 but for an averaging timescale $\tau = 0.5$ year.

Figure S12. Same as Figure S7 but for an averaging timescale $\tau = 1$ year.
Table S5. Same Table S1 for the ratio \(<P_a>/<P_a>_{t=1yr}\) for the estimated power input into the magnetosphere, \(P_a\)

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<td>-159.387</td>
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**Figure S13.** Same as Figure S1 but for the ratio $\langle P_\alpha \rangle / \langle P_\alpha \rangle_{\tau=1yr}$ for the estimated power input into the magnetosphere, $P_\alpha$ (and for an averaging timescale $\tau = 3$ hours).

**Figure S14.** Same as Figure S13 but for an averaging timescale $\tau = 1$ day.
Figure S15. Same as Figure S13 but for an averaging timescale $\tau = 7$ days

Figure S16. Same as Figure S13 but for an averaging timescale $\tau = 27$ days
Figure S17. Same as Figure S13 but for an averaging timescale $\tau = 0.5$ year.

Figure S18. Same as Figure S13 but for an averaging timescale $\tau = 1$ year.
Part 3. List of largest storms in rank order defined by 24-hour running means of corrected $ap$ values, $Ap_C^*$

As pointed out by Allen [1982], taking means over each calendar day is not appropriate when identifying a geomagnetic storm because any storm that straddles 24 hrs UT would be recorded as two moderately-active days rather than a single storm. Hence, daily mean $ap$ (i.e., $Ap$) values are not appropriate and we here employ Allen’s idea of using 8-point running (boxcar) means over all 24-hour intervals, termed $Ap^*$, as has also been used by Kappenman [2005] and Cliver and Svalgaard [2004].

However, we also make corrections to the $ap$ values. Our recent research on the collective response of networks of stations contributing to geomagnetic indices has shown that the $ap$ index tends, on average, to exaggerate the semi-annual variation in geomagnetic activity and has a low response in northern-hemisphere winter [Lockwood, M., A. Chambodut, I. D. Finch, L. A. Barnard, and M. J. Owens (2019) Time-of-day / time-of-year response functions of planetary geomagnetic indices, to be submitted to J. Space Weather Space Clim.]. Lockwood et al. [2018d, e] have made corrections to the $aa$ geomagnetic index and our work on the response functions of the various mid-latitude range indices employs the model that was developed for that work. This research reveals that the $am$ geomagnetic index has a very flat, almost ideal, time-of-day/time-of-year response at all activity levels because it employs relatively uniform rings of mid-latitude stations in both hemispheres and uses weighted means to account for any spatial non-uniformity of the station network. Cliver and Svalgaard [2004] recognized the quality of the $am$ index, compared to indices derived from a less-ideal distribution of stations, and used it to correct for the false time-of-day variation in the $aa$ index (and so created what they termed $Aa_m$). However, they did not correct for the associated false time-of-year variation in $aa$ [Lockwood et al., 2018e]. They then used the Allen [1982] suggestion of 24-hour running means of $Aa_m$ (which they termed $Aa_m^*$) which largely suppresses the false time-of-day variation anyway. We here apply the same philosophy that Cliver and Svalgaard [2004] adopted, but use $am$ to correct for the false time-of-year variation in $ap$. We do this because the $am$ index data only extends back to 1959 whereas the $ap$ index is available from 1932 onward.

The $ap$ index is compiled from a network of stations that is predominantly in the northern hemisphere, with many in Europe. The compilation of the $ap$ index employs station- and activity-dependent “look-up tables” to convert the data from a station into a form that matches that from the Niemegk reference station before averaging them. Our research shows that this causes $ap$ to slightly exaggerate the average semi-annual variation and gives a poorer response in northern-hemisphere winter compared to $am$. However, the effect is complex and depends on the level of geomagnetic activity. We here employ a corrected $ap$ index, $ap_{C_r}$, which allows for these effects as a function of the fraction of each year ($F$) using the formula

$$ap_{C_r}(F) = ap(F) \times C_{ap}(F, ap)$$

where $C_{ap}(F, ap) = (<am(F, ap)_>bin / <am>_all) / (<ap(F, ap)>bin / <ap>_all)$

$$= (<am(F, ap)>bin / <ap(F, ap)>bin) \times (<ap>_all / <am>_all)$$

where the subscript “all” refers to the averaging of all co-incident $ap$ and $am$ data for 1959-2017 (inclusive) and the subscript “bin” refers to the averaging of data in a given $F$ and $ap$ bin for the same interval. Multiplying by the ratio of the all-over means of $ap$ and $am$ means that we correct for the
variation with \( F \) but do not change the average levels of \( ap \). In practice, the data were divided into 40 percentiles of the overall \( ap \) distribution giving 6282 samples in each \( ap \) bin, the values of \( C_{ap}(F,ap) \) were then fitted with a 6th order polynomial in \( F \). Note that we are not concerned with any limitations in the UT dependence of the response of \( ap \) because we use averages over 24-hour intervals, \( Ap_{C^*} \). Further details are given in Appendix A of the main paper. We note that this correction is only approximate because the network of stations used to generate the \( ap \) index has changed a number of times since 1932. However, we do not find any major discontinuities in the derived \( C_{ap}(F,ap) \) at any of these changes since 1959 and so use the assumption that effects of changes before this date also have negligible effect.

We then follow the procedure of Allen [1982] to make 24-hour boxcar means of \( ap_{C^*} \), \( Ap_{C^*} \). For the purposes of identifying and ranking storm days we take the largest value of the 8 such running-means in each calendar day \( [Ap_{C^*}]_{MAX} \). The 100 largest values of \( [Ap_{C^*}]_{MAX} \) since 1932 are given in Table S7 in rank order. Although there are similarities, this list has a somewhat different ranking order to previous studies [e.g., Nevanlinna et al., 2006; Kappenman, 2005; Cliver and Svalgaard, 2004], largely because we have made allowance for the variation of \( ap \) response with time of year. Note that even quite small changes in the estimated magnitude of the storm day can have a large effect on its ranking order.

In the table “est.” means estimated rather than directly observed: these events (listed in italics) are not included in the rank order but are listed to act as context. The “estimate 2”, \( [Ap^*]_{MAX} \) values are taken to be 296±16 for both the Carrington (03 September1859) and STEREO (23 July 2012) events and have not been subject to the same correction for time of year as the observed \( ap \) estimates. Also given are values for these events that have been corrected (“estimate 1”, \( [ Ap_{C^*}]_{MAX} \) values) of 224±12 and 221±12, which drops them both down the ranking order by several places). The rationale that this correction is required for these estimated event sizes is discussed in the main text. Note that all these values come from Cliver and Svalgaard’s [2004] estimate of a peak of \( Aa^* = 425nT \) for the Carrington event and we do not here attempt to estimate, or employ, uncertainties on that estimate – we simply evaluate its consequences for the likely \( Ap^* \) and \( Ap_{C^*} \) values.
Table S7. Storm days ranked by the largest value of the 8-point (1 day) boxcar smoothed mean in the day ([ApC*]_{MAX}) of ap C, the ap geomagnetic index that has been corrected to allow for its time-of-year dependence. The value of [ApC*]_{MAX} as a ratio of the annual mean for the calendar year in question is also given for each storm day. The coloured symbols in column 1 are the same as used in Figure 2 of main text.

<table>
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<tr>
<th>Date</th>
<th>Sun-spot cycle</th>
<th>Cycle-phase (%)</th>
<th>Notes: event name, notable features, and references</th>
<th>[ApC*]_{MAX}</th>
<th>[ApC*]<em>{MAX} / &lt;apC&gt;</em>{1year}</th>
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<td>03 September 1859</td>
<td>9</td>
<td>104 Peak of “Carrington” event [1,45,46,48]</td>
<td>284±30</td>
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<tr>
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The remaining 30947 daily \(A_p c^{*}\)\text{MAX} values (97.68% of all available values for 1932-2017, inclusive)

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