

Forecasting Solar Flares and Coronal Mass Ejections (CMEs)

I. Scene-setting and Overarching Considerations

Manolis K. Georgoulis*

Space Exploration Sector, Johns Hopkins APL, Laurel, MD

*(on leave of absence) RCAAM of the Academy of Athens, Greece

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Operational Space Weather Fundamentals



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Outline

□ What are flares and CMEs? A practical guide

□ Forecasting is a generic task

□ The full set of extreme solar weather problems

□ Forecast how-to

□ Assessing forecast quality: verification & validation

□ The era of machine learning

Conclusions – Part I

A tale of two solar active regions: which one is the "bad" one?

NOAA AR 11093, Aug 2010



NOAA AR 11158, Feb 2011

- > The one on the right was way more flaring than the one on the left
- If you guessed the one on the right, good for you!

Now, quantify your lucky guess.

Solar flares: what are they?

Solar flare (American Heritage Dictionary): a sudden eruption of magnetic energy released on or near the surface of the Sun, usually associated with sunspots and accompanied by bursts of electromagnetic radiation and particles



2011-08-09T06:00:00 - 12:00:00

Major flares stem exclusively from solar active regions (sunspot complexes)



- Not all sunspots give major flares
- However, the ones that do, tend to manifest intervals of dramatic evolution caused by magnetic flux emergence

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Increasing and decreasing sunspot occurrence frequencies are the base of the solar magnetic cycle



Sunspot observations are intertwined with the invention of telescope (early 1600s). The first flare, however, was observed in 1859



Coronal mass ejections (CMEs): what are they?

Coronal Mass Ejection (American Heritage Dictionary): a massive, bubble-shaped burst of plasma expanding outward from the Sun's corona, in which large amounts of superheated particles are emitted at nearly the speed of light





A mesmerizing view of 22 years of CME activity

NASA Scientific Visualization Studio

Flares vs. CMEs

The NOAA (National Oceanic and Atmospheric Administration) classifies flares logarithmically via their peak photon flux at the 1 - 8 Å spectral range. Therefore,

In active regions, flares

occur without flares

(eruptive flares)

can occur without CMEs

(confined). CMEs cannot

In the quiet Sun (beyond

occur without major flares

active regions), CMEs

The larger the flare, the

more likely it is to be

eruptive (i.e., CME-

associated)

debated

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Flare Class	Peak photon flux at 1-8 A (W/m²)
А	10 ⁻⁸
В	10 ⁻⁷
С	10 ⁻⁶
М	10 ⁻⁵
Х	10-4
X10	10 ⁻³

Already from C-class and above, flares virtually occur exclusively in active regions

- \blacktriangleright CMEs can be slow (speed < (750 900) km/s) or fast, when their speed is above that limit. Their speed can reach values > 3000 km/s
- CMEs can occur both in active regions and in the quiet Sun
- 1.0 0.8 CME association rate 0.2 Results published by Yashiro et al., (2005) **GOES flare class** 0.0 х 10-4 10-5 10 Flare ppf (W/m²) What causes what, however, is

Yashiro et all., ApJ, 2005; Anastasiadis et al., SoPh, 2017

Early observations of flares and the seeds for forecasting



Major changes and loss of magnetic energy before and after a 'great' flare of July 16, 1959 (Mt. Wilson & Crimean Observatory)



Plotting the number of flare events vs. their sizes, one sees very well-defined straight lines in log-log plots. These power laws indicate self-similarity



Zirin & Liggett, SoPh, 1987

The more complex the sunspot, the more likely to be associated with flares. Picture of a " δ -sunspot" above, associated with a great flare

- Major flares & shear (Hagyard et al., SoPh, 1984)
- Sunspot classes & flares (McIntosh, SoPh, 1990)

Flares as Poisson processes



Rosner & Vaiana, ApJ, 1978

Flares are:

- Stochastic relaxation (storage and release) processes
- Physically uncoupled / independent from each other
- Brief, compared to intermediate times between them.

Hence, their probability of occurrence at time t is

$$P(t) = \bar{\nu}e^{\bar{\nu}t}$$

This can lead to a power-law occurrence frequency for flare energies

$$P(E) \sim (1 + \frac{E}{E_0})^{-\gamma}$$

Oh, the irony: instabilities triggered in a self-organized or SOC system are stochastically triggered, and so hardly predictable

Credit: Christensen & Moloney (2005)



Power laws are often attributed to selforganized critical (SOC) phenomena, aka 'avalanches' of energy release

What is prediction?



Refresh

- By looking at an instantaneous value or a timeseries of condition(s) / parameter(s) of choice, determine (by a Boolean 1 [YES] or 0 [NO] or a probability ∈ (0,1)) whether an event (any event) of a preset size will occur within a preset prediction window. Need to specify:
 - Predictive model using single or multiple parameters
 - Flare size (typically by NOAA/GOES class)
 - Prediction window
 - Observation window or not (point-in-time)
 - Latency, if any
 - Refresh rate

Define. Predict. Repeat.

What is an operational (solar weather) forecast?

- A forecast mechanism or infrastructure that works 24/7, 365/12 with or without human intervention
- Continuous monitoring of the Sun (the earthward solar hemisphere) and a forecast for the pre-defined events that is existing any time
- Humans on duty, or "humans in the loop" at any given time, to answer questions and provide information / support
- Who is forecasting flares today?
 - Space Agencies around the world
 - Companies / startups / contractors
 - Research teams / academics
- Who is forecasting CMEs (before they occur) today?
 - Much fewer entities, mainly research teams / academics
- Operational missions for operational forecasting? Not so many.



Solar weather (the solar end of space weather) at a glance



The full set of solar weather problems

➢ In the higher-energy solar events, we have flares, CMEs and SEP events





How to forecast

One needs data to <u>train</u>, <u>validate</u>, and <u>test</u> a forecast



- Out of a multitude of existing data, one chooses three (i) homogeneous, (ii) non-overlapping by any means and (iii) statistically significant / representative samples
- The training sample is typically one of known* (labeled) input and output (event / no event) instances
- The validation sample is typically one of known (labeled) input and output instances, but the output is treated as unknown and the forecast result is compared to it
- The testing sample is a sample of inputs with unknown outputs, near-real time in operational settings. The prediction is issued and then checked a posteriori, i.e., after the prediction window

* Save for unsupervised and deep learning methods

On what samples?

> Solar magnetic fields (data) and related physics-based metadata have the lion's share

Keyword	Description	Unit ¹	Formula ²	Statistic	Error Keyword	Data Sourc
USFLUX	Total unsigned flux	Мx	$\Phi = \sum B_z dA$	Integral	ERRVF	SWPC
MEANGAM	Mean angle of field from radial	Degree	$\overline{\gamma} = \frac{1}{N} \sum \arctan \left(\frac{Bh}{B_z} \right)$	Mean	ERRGAM	1221 12
MEANGBT	Horizontal gradient of total field	${ m GMm^{-1}}$	$ \nabla B_{\rm tot} = \frac{1}{N} \sum \sqrt{\left(\frac{\partial B}{\partial x}\right)^2 + \left(\frac{\partial B}{\partial y}\right)^2}$	Mean	ERRBT	Catalogues Surface-no
MEANGBZ	Horizontal gradient of ver- tical field	${\rm GMm^{-1}}$	$ \nabla B_z = \frac{1}{N} \sum \sqrt{\left(\frac{\partial B_z}{\partial x}\right)^2 + \left(\frac{\partial B_z}{\partial y}\right)^2}$	Mean	ERRBZ	and line-of magnetogr
MEANGBH	Horizontal gradient of hor- izontal field	${ m GMm^{-1}}$	$\overline{ \nabla B_h } = \frac{1}{N} \sum \sqrt{\left(\frac{\partial B_h}{\partial x}\right)^2 + \left(\frac{\partial B_h}{\partial y}\right)^2}$	Mean	ERRBH	
MEANJZD	Vertical current density	$\mathrm{mAm^{-2}}$	$\overline{J_z} \propto \frac{1}{N} \sum \left(\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right)$	Mean	ERRJZ	
TOTUSJZ	Total unsigned vertical current	А	$J_{z_{total}} = \sum J_z dA$	Integral	ERRUSI	
MEANALP	Characteristic twist parameter, α	Mm ⁻¹	$\alpha_{total} \propto \frac{\sum J_z \cdot B_z}{\sum B_z^2}$	Mean	ERRALP	
MEANJZH	Current helicity $(B_z \text{ contribution})$	$\mathrm{G}^{2}\mathrm{m}^{-1}$	$\overline{H_c} \propto \frac{1}{N} \sum B_z \cdot J_z$	Mean	ERRMIH	
TOTUSJH	Total unsigned current he- licity	$\mathrm{G}^{2}\mathrm{m}^{-1}$	$H_{e_{total}} \propto \sum B_z \cdot J_z $	Sum	ERRTUI	
ABSNJZH	Absolute value of the net current helicity	$\mathrm{G}^{2}\mathrm{m}^{-1}$	$H_{c_{abs}} \propto \sum B_z \cdot J_z $	Sum	ERRTAI	
SAVNCPP	Sum of the modulus of the net current per polarity	А	$J_{z_{sum}} \propto \left \sum_{z}^{B_z^+} J_z dA \right + \left \sum_{z}^{B_z^-} J_z dA \right $	Integral	ERRJHT	Full-vector magnetogr
MEANPOT	Proxy for mean photo- spheric excess magnetic en- ergy density	erg cm ⁻³	$p \propto \frac{1}{N} \sum \left(\boldsymbol{B}^{\text{Obs}} - \boldsymbol{B}^{\text{Pot}} \right)^2$	Mean	ERRMPOT	
тотрот	Proxy for total photo- spheric magnetic free en- ergy density	$\rm erg cm^{-1}$	$\rho_{\rm tot} \propto \sum \left({{{{\vec B}^{\rm Obs}} - {{\vec B}^{\rm Pot}}} \right)^2 dA$	Integral	ERRIPOT	
MEANSHR	Shear angle	Degree	$\overline{\Gamma} = \frac{1}{N} \sum \arccos \left(\frac{B^{\text{Obs}} \cdot B^{\text{Pot}}}{ B^{\text{Obs}} B^{\text{Pot}} } \right)$	Mean	ERRMSHA	
shrgt45	Fractional of Area with		Area with Shear $> 45^{\circ}$ / HARP Area	Fraction		Intensity in
	Shear $> 45^{\circ}$		Bobra et al.,	SoPh, 2	2014	-
				/		

Data Source	Property group	No. of predictors	Relevant predictor	Adapted from	Related references
SWPC	Solar region summary (SRS) properties	2	McIntosh and Hale classes	McCloskey et al. (2016)	McIntosh (1990)
		3	Number, area and longitudinal extend of sunspots		Lee et al. (2012)
Catalogues	GOES soft X-ray flare events ^{a,b}	4	Flare magnitude, start, peak, and end times		
Surface-normal component (radial and line-of-sight)	Effective connected magnetic field strength ^c	1	B _{eff}	Georgoulis & Rust (2007), Georgoulis (2011, 2013)	
magnetograms	Fractal and multifractal parameters	1	Fractal dimension	Conlon et al. (2008)	Abramenko et al. (2003)
		1	Generalized correlation dimension		Abramenko (2005)
		2	Holder exponent; Hausdorff dimension		Al-Ghraibah et al. (2015)
		2	Structure function's inertial range index		
	Fourier and Wavelet power spectral indices	2	Power-law exponent	Hewett et al. (2008), Guerra et al. (2015)	
	Decay index (DI) ^d	8	Mean DI over PIL segments; height of DI; ratio of PIL length to DI height	Liu (2008) Zuccarello et al. (2014)	
	Magnetic PIL properties	5	Sum of PIL segments, longest PIL segment	Mason & Hoeksema (2010)	
	•	1	R value	Schrijver (2007)	
		1	WL _{sg}	Falconer et al. (2012)	
	3D magnetic null points ^d	6	Number of null points in different height ranges (from 2 to 100 Mm above photosphere)	Haynes & Parnell (2007)	Pontin et al. (2013) Barnes & Leka (2006)
	Ising Energy ^c	6	Original and partitioned Ising energy	Ahmed et al. (2010)	Kontogiannis et al. (2018)
	Magnetic energy and helicity	11	Poynting flux and magnetic helicity flux proxies	Park et al. (2010) Park et al. (2012)	
Full-vector magnetograms	SHARP properties ^e	100	Horizontal gradient of <i>B</i> components; shear angle; unsigned vertical current; higher-order moments of time series	Bobra et al. (2014) (validated) Leka & Barnes (2003b, 2007)	
	Magnetic energy and helicity	22	Poynting flux and magnetic helicity flux	Kusano et al. (2002)	Berger & Field (1984), Welsch et al. (2009)
	Non-neutralized currents	6	Total non-neutralized current	Georgoulis et al. (2012)	Kontogiannis et al. (2017)
	Flows around PIL	22	Speed of diverging/converging/shear flows	Park et al. (2018)	Deng et al. (2006), Wang et al. (2014)
Intensity images ^f	Magnetic field gradient	3	Total horizontal magnetic gradient	Korsós et al. (2014)	Kontogiannis et al. (2018)

Georgoulis et al., JSWSC, 2021

On what samples?

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Talk I. Scene-Setting & Overarching Considerations

And what methods?

There are mainly four broad classes of prediction methods

Physics-based

Statistical

Ensemble

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APL

> AI / Machine Learning

Mainly self-organized criticality / sandpile models

Fractal / multifractal; Bayesian; discriminant analysis; SEA; best fit; decision boundary; Poisson

Supervised; unsupervised; hybrid; reinforcement; deep

Combining methods or probabilities





TOOLBOX"

TYPES OF MACHINE LEARNING





Performance verification: assessing forecast quality

- Performance verification: how well (or bad) my method works?
- > <u>Validation</u>: how does it compare to other methods aiming to predict the same task?

Binary (dichotomous) forecasting

Q: Will an event of given specs happen within the given time?

A: YES or NO

APL

		Flaring observed		
		Yes	No	
Flaring Predicted	Yes No	True positive (TP) False negative (FN)	False positive (FP) True negative (TN)	

Probabilistic forecasting

Q: What is the probability that an event of given specs will happen within the given time?

A: P ∈ [0,1]

Reliability diagram: observed frequency vs. forecast probability



Key metrics and skill scores

Binary (dichotomous) forecasting

Name	Notation	Formula	Range
Accuracy	ACC	$\frac{\text{TP} + \text{TN}}{N}$	[0, 1]
False alarm ratio	FAR	$\frac{FP}{TP + FP}$	[0, 1]
Bias	BIAS	$\frac{\mathrm{TP}+\mathrm{FP}}{\mathrm{TP}+\mathrm{FN}}$	[0, ∞]
Threat score	TS	$\frac{TP}{TP + FN + FP}$	[0, 1]
Equitable threat score	ETS	$\frac{\text{TP} - R_{\text{ETS}}}{\text{TP} + \text{FN} + \text{FP} - R_{\text{ETS}}}$	$[-\frac{1}{3}, 1]$
		Using $R_{\text{ETS}} = \frac{(\text{TP} + \text{FN})(\text{TP} + \text{FP})}{N}$	
Probability of detection	POD	$\frac{TP}{TP + FN}$	[0, 1]
Probability of false detection	POFD	$\frac{FP}{FP + TN}$	[0, 1]
Odds ratio	OR	$\frac{\text{TP} \cdot \text{TN}}{\text{FN} \cdot \text{FP}}$	[0, ∞]
Odds ratio skill score	ORSS	$\frac{(\mathrm{TP}\cdot\mathrm{TN})-(\mathrm{FN}\cdot\mathrm{FP})}{(\mathrm{TP}\cdot\mathrm{TN})+(\mathrm{FN}\cdot\mathrm{FP})}$	[-1, 1]
Heidke skill score	HSS	$\frac{\text{TP} + \text{TN} - R_{\text{HSS}}}{N - R_{\text{HSS}}}$	[-1, 1]
		Using $R_{\text{HSS}} = \frac{(\text{TP} + \text{FN})(\text{TP} + \text{FP}) + (\text{TN} + \text{FN})(\text{TN} + \text{FP})}{N}$	
True skill statistic	TSS	POD – POFD	[-1, 1]
Symmetric extremal dependence index	SEDI	$\frac{\log(\text{POFD}) - \log(\text{POD}) - \log(1 - \text{POFD}) + \log(1 - \text{POD})}{\log(\text{POFD}) + \log(\text{POD}) + \log(1 - \text{POFD}) + \log(1 - \text{POD})}$	[-1, 1]
Appleman's discriminant	AD	$\frac{\text{TN} - \text{FN}}{\text{FP} + \text{TN}} \text{ if (TP + FN) > (FP + TN)}$	[- <u>FN</u> , 1]
		$\frac{\text{TP} - \text{FP}}{\text{If}}$ if (TP + FN) < (FP + TN)	[- <u>FP</u> , 1]

Probabilistic forecasting

Brier score:

$$BS = \frac{1}{N} \sum_{i=1}^{N} (o_i - p_i)^2 \qquad o_m \equiv 0, 1$$
$$p_m \in (0, 1)$$

Reference score (climatology):

$$BS_{ref} = \frac{1}{N} \sum_{i=1}^{N} (o_i - \bar{o})^2 \quad \bar{o} = \frac{1}{N} \sum_{i=1}^{N} o_i$$

Brier skill score:

$$BSS = 1 - \frac{BS}{BS_{ref}}$$

Finds how close the probabilistic forecasting is to binary forecasting (very stringent test)

Key metrics and skill scores

Binary (dichotomous) forecasting

Heidke skill score	HSS	$\frac{\text{TP} + \text{TN} - R_{\text{HSS}}}{N - R_{\text{HSS}}}$	[-1, 1]
		Using $R_{\text{HSS}} = \frac{(\text{TP} + \text{FN})(\text{TP} + \text{FP}) + (\text{TN} + \text{FN})(\text{TN} + \text{FP})}{N}$	
True skill statistic	TSS	POD – POFD	[-1, 1]
Symmetric extremal dependence index	SEDI	$\frac{\log(\text{POFD}) - \log(\text{POD}) - \log(1 - \text{POFD}) + \log(1 - \text{POD})}{\log(\text{POFD}) + \log(\text{POD}) + \log(1 - \text{POFD}) + \log(1 - \text{POD})}$	[-1, 1]
Appleman's discriminant	AD	$\frac{\text{TN} - \text{FN}}{\text{FP} + \text{TN}} \text{ if (TP + FN) > (FP + TN)}$	$\left[-\frac{\text{FN}}{\text{FP}}, 1\right]$
		$\frac{\mathrm{TP}-\mathrm{FP}}{\mathrm{FN}+\mathrm{TP}} \text{ if } (\mathrm{TP}+\mathrm{FN}) < (\mathrm{FP}+\mathrm{TN})$	[- <u>FP</u> , 1]

Operations-to-Research and the R2O-O2R loop

- Successive iterations optimizing research and operations
 - Physics-based (research) parameters are routinely used for SWx prediction (operations)



Can first-attempt operations be improved, and how?



By achieving interpretable results that can then be fed into improved (optimized) research

Some simple, early ideas: Poisson forecasting

From the Poisson distribution, the probability of observing k flares per unit time interval is

 $P_{\ell}(k) = \frac{\ell^k}{k!} e^{-\ell}$

the number of eventsexpected per unit interval

➤ The probability of getting <u>at least one flare</u> $(k \ge 1)$ is

$$P_{\ell}(k \ge 1) = 1 - P_{\ell}(k = 0)$$

> Because $P_{\ell}(k=0) = e^{-\ell}$, having an idea of ℓ , we obtain

 $P_{\ell}(k \ge 1) = 1 - e^{-\ell}$

Working on the expected rate of flares in case a certain sunspot class arises (McIntosh, SoPh, 1990)

www.SelarMenitor.org







Some simple, early ideas: Bayesian reasoning

> Bayes' theorem:



(Simplified) Laplace's rule of succession

$$p_{thres} = \frac{\mathcal{F} + 1}{k + 2} \quad \delta p_{thres} = \sqrt{\frac{p_{thres}(1 - p_{thres})}{k + 3}}$$

- P_{thres}: the flare probability if the predictor exceeds a certain threshold
- *F*: number of predictor values above the threshold that were associated with a flare
- k total number of predictor values above threshold

Jaynes 2003; Wheatland, PASA, 2005; Georgoulis, SoPh, 2012



AI / ML and DL in forecasting: why using them?

- > The objective is to distinguish between eventful and uneventful parts of the distribution in parameter space
- > Each dimension of the parameter space is one of the predictors (so we are talking about 10s and 100s of dimensions)
- > **Dimensionality reduction:** from full n-dimension hypervolumes to n' < n –dimension hypersurfaces



van der Maaten et al., 2009

Machine Learning

A definition: Machine learning is a natural outgrowth of the intersection of Computer Science and Statistics that seeks to answer the following question:

'How can we build computer systems that automatically improve with experience, and what are the fundamental laws that govern all learning processes?'

Tom M. Mitchell's 'The Discipline of Machine Learning' (Carnegie Mellon U., 2006)

Machine learning can be:

- > **Supervised:** trained on labeled samples
- Unsupervised: trained on unlabeled samples
- Hybrid: combining both elements, training on data that can be both labeled and unlabeled



Deep Learning

A definition: Deep Learning is a particular kind of machine learning that achieves great power and flexibility by representing the world as a nested hierarchy of concepts, with each concept defined in relation to simpler concepts, and more abstract representations computed in terms of less abstract ones.

Goodfellow, Bengio & Courville's 'Deep Learning' (MIT Press, 2016)

Unsupervised, and hence hard to interpret

Two questions of capital importance:

- Do we have enough data for DL applications?
- ➢ How to interpret?

Why deep learning?



Credit: Andrew Ng

Interpretability of performance: how to?

- In non-interpretable models, including DL, you can forger about parameter ranking
- Hard to interpret why a classification can be radically different



Fig. 2 | Saliency does not explain anything except where the network is looking. We have no idea why this image is labelled as either a dog or a musical instrument when considering only saliency. The explanations look essentially the same for both classes. Credit: Chaofen Chen, Duke University

Rudin, Nat.Intel., 2019

In more human-sensitive decisions, ethical problems

appear

machine intelligence

Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead

Cynthia Rudin

PERSPECTIVE



But SWx prediction will soon become a human-sensitive issue, as well



A potential hope: physics-informed neural networks and similar methodologies

Neural Networks trained to solve supervised learning tasks while respecting any given laws of physics described by general nonlinear partial differential equations, Raissi et al., J. Comp. Phys., 2019



Karniadakis et al., Nature Rev./Physics, 2021

PINNs as PDE solvers: PINNs are yet to be applied for SWx forecasting, but have been recently used successfully for ultra-fast NLFF field extrapolations!



Jarolim et al., Nat. Astron., 2023

Conclusions – Part I

- We discussed the problem of prediction of solar flares and CMEs and the methods applied to this problem
- One key element of the problem is interdisciplinarity: solar weather prediction is too important a business to be left to solar physicists alone
- □ Forecasts (any forecasts) cannot stand without a robust assessment of their quality
- □ R2O and O2R are pursuits of capital importance. Their loop (R2O ← → O2R) is essentially an optimization loop and is based on, and feeds from, physical interpretation
- Machine and deep learning are prime tools on this, but we are lacking on interpretation. Hence, the R2O – O2R loop is still not achieved sufficiently
- Methodologies such as PINNs, Physics-Enhanced Deep Surrogates (PEDS), etc. can be a key to achieving the R2O – O2R loop
- Success or failure of ML/DL interpretability will depend on their success to be used as solvers of partial differential equations. Space physics is built around PDEs.



JOHNS HOPKINS APPLIED PHYSICS LABORATORY

Questions / comments: manolis.georgoulis@jhuapl.edu

BACKUP INFORMATION

