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INVITED

Estimating and predicting atmospheric stability for safe agricultural spraying of pesticides

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Abstract: Modern farming and agriculture commonly use pesticide sprays to efficiently manage on-farm operations. 'Spray drift' is defined as the movement of pesticide outside the target spray area. Long-distance spray drift is a big problem causing millions of dollars in economic losses each year due to damage to crops from off-target spray. There are also unknown human health implications as regional communities, rainwater tanks and the surrounding natural environment are contaminated by off-target pesticides via spray drift.

Grace & Tepper (2021) established a link between atmospheric stability and the standard deviation of vertical wind direction (sigma w). Sigma w (or an estimate) is likely to be a better indicator of hazardous and non-hazardous spay conditions compared to the more standard use of thermal air inversions which can be overly prohibitive. Sigma w can be directly measured by 3-dimensional sonic wind anemometers, but the cost can be prohibitive. Most of the COtL Mesonet weather stations in South Australia (SA) do not directly measure sigma w, but are fitted with a range of other meteorological sensors. The objective of this study is to assess, via machine learning, the performance of estimating real-time sigma w from other on-site meteorological data.

A logistic Artificial Neural Network (ANN) with outputs of a binary nature was optimised for a sigma w threshold value of 0.2 m/s. This threshold value for sigma w corresponds to hazardous spray conditions and represents a danger for long-distance spray drift to occur (Grace & Tepper, 2021). For a comparative check, a multivariate regression algorithm for sigma w was also developed which was informed by Monin-Obukhov Stability Theory.

The ANN was trained on five specialised 'Research weather stations' in South Australia with approximately one to two years of 10-minutely data. The resultant ANN performed very well with a Hit Rate of 99%, a False Alarm rate of 9% and an overall 93% proportion correct. This compares favourably to the Monin-Obukhov Stability Theory informed multivariate regression algorithm (Hit Rate of 81%), and compares very favourably to the current regulations which ban spraying during any inversion (i.e. assuming sigma w < 0.2 m/s for all thermal inversions has a False Alarm rate of 38%). In addition to the various performance metrics, example 48-hour time period charts show the ANN has excellence performance.

A logistic ANN was also optimised to provide predictions for farmers for two hours into the future. A 2-hour safe spray window prediction is very useful to spray applicators and growers. It performed reasonably well with a Hit Rate of 93% and a False Alarm Rate of 16%.

These algorithms can be used for the COtL Mesonet which covers the Mid North and Riverland/Mallee regions of SA and would be very beneficial for efficient farm management and to reduce pesticide pollution.

Keywords: *Spray drift, hazardous inversion detection, Mesonet, sigma w, agriculture*

1. INTRODUCTION

1.1. General spray drift background

Many agricultural regions commonly use pesticide sprays to efficiently manage their farms. Spray drift is defined as the movement of droplets outside the target spray area. This is a problem as spray drift can cause:

- damage to off-target sites (such as another farmer's crops)
- damage to market demand for products highly sensitive to detectable pesticide residue (i.e. organic farms, wine exports to China)
- environmental and residential garden contamination;
- drinking water and rain-tank contamination and
- insufficient pesticide over the target crop and the pesticide and application labour is wasted.

One of the main components affecting spray drift is the weather conditions at the time of spraying. Specifically, very stable weather conditions increase the likelihood of long-distance spray drift, whereby the pesticides can float in the air and settle down up to 100km away from the target crop. Such stable conditions are generally caused by an 'inversion' whereby a layer of warmer air sits above cooler air at the ground surface. According to the Australian Pesticides and Veterinary Medicines Authority (APVMA), spraying of pesticides should not be done if there are 'hazardous surface temperature inversions present' (APVMA, 2019). It is illegal to spray during a hazardous inversion, and unless otherwise shown, all inversions must be considered hazardous. Before the COtL Mesonet was installed in 2019, it was very difficult for farmers to assess objectively when an inversion was occurring, let alone whether it was hazardous or not. A rule of thumb had been to avoid spraying between 2 hours before sunset and 2 hours after sunrise, however this is overly restrictive and hence did not garner meaningful compliance. With the installation of the COtL Mesonet, real-time inversion detection was provided, yet this is still viewed as too restrictive by many in the agricultural sector.

Grace & Tepper (2021) established a link between atmospheric stability and the standard deviation of vertical wind speed (sigma w). Sigma w (or an estimate) is a better indicator of hazardous and non-hazardous spay conditions compared to the more conventional use of vertical temperature differences (i.e. presence of an inversion) which can be overly prohibitive. That is, whether sigma w is above or below an associated threshold value can be used as a proxy for hazardous and non-hazardous spray conditions and provides guidance to spray applicators to avoid spray drift damage. Allowing farmers to spray during non-hazardous inversions (based on the sigma w value) would allow better flexibility in farm management practices, better compliance and thus better outcomes for the community and environment.

Sigma w is directly measured by 3-dimensional sonic wind anemometers, but the cost can be prohibitive. Most stations within the COtL Mesonet in South Australia (SA) do not directly measure sigma w but are fitted with a range of other meteorological sensors. This paper details the assessment of using artificial neural networks (ANNs) to estimate real-time sigma w from other meteorological data, and hence the possibility of applying it to existing weather station networks.

2. DATA SUMMARY

Five of the 71 Automatic Weather Stations (AWS) in the COtL Mesonet were suitable for use in this study and are located in South Australia. The Mid North region contains three 'Research Stations' equipped with 3D sonic wind anemometers at a height of 10 metres, and the Riverland / Mallee region contains two 'Research Stations'.

2.1. Data collation and selection

In addition to 3-dimensional sonic wind anemometers at 10m, these Research Stations also have temperature, pressure and humidity sensors at 1.2m, 2-dimensional sonic wind anemometers at 2m, a vertical temperature difference measurement (between 10m and 1.2m), a pyranometer sensor and a tipping bucket rain gauge.

The data from the five Research Stations generally spanned across early 2020 though to mid-2022, reported in 10-minute timesteps. Combined, there are over 250,000 data points (all time steps and all stations). A summary of the data from these stations is in Table 1.

All the data available was trialled in this study. The data also included micrometeorological variables such as Richardson number, friction velocity, skew and kurtosis of horizontal wind speed components and estimates of surface drag coefficients which vary by location and crop and pasture stage. Where appropriate, the aforementioned micrometeorological data were transformed to an appropriate range. The changes in each variable over time and 'polynomialised' combinations of variables were also included. Preliminary investigations showed that not all variables significantly affected the model performance, and hence to reduce computing load, not all variables were included for the ANN. Over 450 input variables were used for the ANN.

Table 1. Summary of data used for this study

Location	ID	Start Date	End Date	Period
Wandereah East, SA	06	Jul 2021	Jul 2022	~ 1 year
Hart, SA	18	Feb 2020	Jul 2022	~ 2.5 years
Korunye, SA	36	Jan 2022	Jul 2022	~ 0.5 years
Loxton, SA	109	Jun 2021	Jul 2022	~ 1 year
Geranium, SA	126	Jun 2021	Jul 2022	~ 1 year

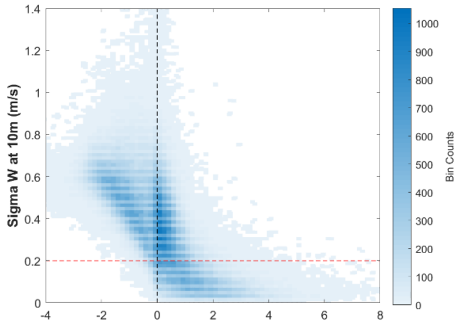

Figure 1. Sigma w against VTD (ºC)

2.2. Sigma W, inversions and sprayable hours

When sigma w is below the threshold of 0.2 m/s, there is almost always a concurrent inversion (i.e. Vertical Temperature Difference (VTD) is positive). Approximately 1% of times, sigma w will be below 0.2 m/s when there is no inversion. This is shown in Figure 1.

Based on October 2022 to March 2023, a defined hazardous condition of sigma w < 0.2 would provide on average an additional 3.5 sprayable hours per 24-hour-day compared to solely using inversions (VTD>0) as guidance. This refined definition of hazardous conditions would provide on average an additional 10 sprayable hours per 24-hour-day compared to the general rule of thumb of avoiding spraying between 2 hours before sunset and 2 hours after sunrise.

3. ARTIFICIAL NEURAL NETWORKS (ANNS)

Artificial neural networks (ANNs) are a form of machine learning. Machine learning has been shown to produce superior estimates for turbulent surface fluxes as demonstrated by McCandless et al. (2022), and Wulfmeyer et al (2023).

Unlike standard regression models, artificial neural networks have an additional ‘hidden layer’ between the inputs and the outputs. Weights or coefficients are applied to each input before the hidden layer then an activation function is applied within the hidden layer. A second set of weights are then applied to arrive at the output (Figure 2). The Universal Approximation Theorem states that a neural network with one hidden layer can approximate any continuous function for inputs within a specific range.

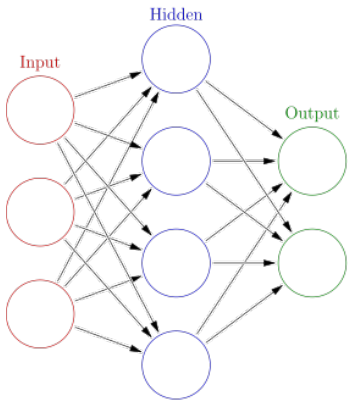

Figure 2. ANN schematic with 1 hidden layer

3.1. Logistic ANNs

A logistic artificial neural network was developed with the below attributes, and the gradient functions set accordingly via feed-forward and back-propagation algorithms. The number of nodes in the hidden layer was set to one less than the number of inputs. The exact value of sigma w is not hugely important compared to whether or not it is above a limiting threshold, hence the measured sigma w values were converted to a binary series of zeros and ones; 0 for values above 0.2, and 1 for values below 0.2 (i.e. hazardous conditions). The overall performance metrics were calculated by rounding the resultant ANN probability outputs to either 0 or 1 and comparing against the measured data.

Activation function: sigmoidal function (also known as ‘logistic function’)

$$g(z) = \frac{1}{1+e^{-z}} \tag{1}$$

Cost function:

$$J(\theta) = \frac{-1}{m}\sum_{i=1}^{m}\left[y_i * \log\left(h_\theta(x_i)\right) + (1-y_i)\log\left(1-h_\theta(x_i)\right)\right] \tag{2}$$

- y = measured sigma w;
- m = total number of measured sigma w values;
- n = number of input variables;
- x = matrix of input variables (m x (n+1));

- $h_{\Theta}(x) = \Theta_{(2)} g(\Theta_{(1)} x^T)$;
- $\Theta_{(1)}$ = matrix of weights corresponding to each input (L x (n+1)), L = number of hidden nodes in hidden layer.
- $\Theta_{(2)}$ = column vector of weights (1 x (L+1)).
- i = i^{th} observation.

4. PERFORMANCE METRICS

The data was split into training, validation and test data to ensure testing was not done using training data. Performance metrics were used to assess whether the model correctly estimates sigma w to be above or below a certain threshold. Table 2 details this and five performance indicators were used based on these binary outputs. In this case, the threshold value is sigma w = 0.2 and the event occurs if sigma w is below the threshold (i.e. the event being unsuitable conditions for spraying).

Table 2. Explanation of performance indicators for binary outputs

		Observed Event		
		Yes	**No**	**Total**
Modelled Event	**Yes**	Hit (a)	False alarm (b)	a + b
	No	Miss (c)	Correct rejection (d)	c + d
	Total	a + c	b + d	n = a + b + c + d

A few simple measures or scores are Hit Rate (H), False Alarm Rate (F), the Critical Success Index (CSI), Yule's Q, and the Proportion Correct (PC).

$$H = \frac{a}{a+c} \tag{3}$$

$$F = \frac{b}{b+d} \tag{4}$$

$$CSI = \frac{a}{a+b+c} \tag{5}$$

$$Q = \frac{ad-bc}{ad+bc} \tag{6}$$

$$PC = \frac{a+d}{a+b+c+d} \tag{7}$$

These definitions are used in many fields such as operations research, medicine, meteorology and signal detection theory although the terminology varies. Ideally, a large H with a small F indicates good performance. In judging the skill of the model, both H and F need to be considered together. Scores such as CSI and Q have the advantage of being single index performance measures and are widely used. CSI is used by many weather agencies for extreme but uncommon events like tornadoes; Q has a maximum of 1 for perfect forecasts and 0 for random forecasts and is recommended by several texts such as Jolliffe & Stephenson (2003).

5. REAL-TIME ESTIMATION OF SIGMA W VIA MULTIVARIATE REGRESSION

Multivariate linear regression was used in conjunction with meteorological judgement to develop an approximation equation for the real-time value of sigma w. This was done to provide a comparative check for the ANN algorithm. Many of the multivariate terms trialled were inspired by the Monin-Obukhov Stability Theory (MOST) such as the bulk Richardson number, friction velocity, and surface roughness.

The performance metrics of this approach are shown in Table 3 (Run C), and achieve a reasonable proportion correct (91%). However, if used in practice, the Hit Rate of 81% means that about 20% of all hazardous spray conditions would be incorrectly classified as safe.

6. REAL-TIME ESTIMATION OF SIGMA W VIA LOGISTIC ANN

Without the use of regularisation, the ANN test errors began to differ to that of the training error after more than 10,000 iterations were conducted. This suggested over-training was occurring. To avoid overtraining, further model runs were trialled using regularisation (optimised for lambda set to 0.2).

Table 3. ANN performance metrics compared to baselines and multivariate regression

Run ID	Trial Run	CSI	Hit Rate	False Alarm Rate	Proportion Correct	Yule's Q
A	Baseline 1: two hours before sunset and two hours after sunrise	0.299	0.993	0.520	0.574	0.985
B	Baseline 2: VTD > 0	0.440	0.948	0.384	0.699	0.934
C	Multivariate regression with meteorological judgement	0.744	0.811	0.042	0.910	0.993
D	Best Logistic ANN with threshold set to 0.25	0.894	0.941	0.024	0.958	0.997
E	Best Logistic ANN with threshold set to 0.25, but assessed against threshold of 0.2	0.781	0.990	0.089	0.931	0.998
F	Best Logistic ANN with threshold set to 0.25, but assessed against threshold of 0.2, and probabilities of 20% to 50% removed as 'caution'.	0.785	0.990	0.089	0.930	0.999

6.1. Results and comparison

The logistic ANN (Run D) resulted in a Hit Rate of 94%, a False Alarm Rate of 2% and an overall proportion correct of 96%. The graph of the training cost and testing cost is shown in Figure 3 and demonstrates that over-training is not occurring. This also shows that there would be no significant benefit if the number of iterations were to be increased.

Given the potential use of these sigma w estimates for spray applicators, it was considered best to add a degree of conservatism into the model. This was done by increasing the threshold to a sigma w value of 0.25 m/s (compared to 0.20 m/s). Furthermore, the raw outputs of the ANN were categorised into three separate categories. Note that the outputs of the logistic ANN are probabilities that sigma w is below the threshold.

- 0% – 20%: Above threshold (safe to spray).
- 20% - 50%: Caution.
- 50% - 100%: Below threshold (hazardous to spray).

When including the aforementioned conservatism, the performance statistics change to a Hit Rate of 99%, a False Alarm Rate of 9% and an overall proportion correct of 93% (Run F). This is significantly better than the performance of the baseline estimations and the estimate from multivariate regression. This is shown in Table 3. The ANN performance is considered sufficiently good to be used in real-world applications.

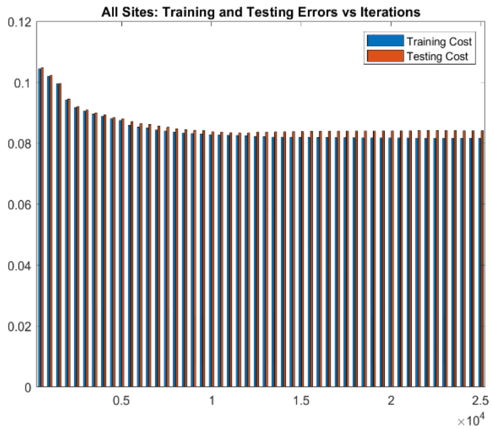

Figure 3. The training and testing errors for an increasing number of iterations (λ=0.2). Although the training cost includes lambda in its total, the testing cost does not. This shows that overtraining is not occurring

6.2. Time and location-specific performance

Performance metrics were investigated based on time of year and also time of day. There was no monthly trend in performance metrics (i.e. the ANN model does not perform differently in summer compared to winter). On an hourly timescale, there was no clear trend in performance metrics either (i.e. the ANN model does not perform differently in mornings compared to evenings). The five locations in SA had slightly varying False Alarm Rates and Hit Rates, but there was no correlation between performance statistics and characteristics of station location.

6.3. Example time-series of real-time estimates

A randomly selected 48-hour time-period for one location illustrates how the optimised real-time ANN algorithm works over a continuous time period (see Figure 4). The measured sigma w values were plotted for the site at Wandearah East, as were the model outputs. The model outputs correspond to Run D/E/F from Table 3 and are the probabilities of sigma w being above or below 0.25 m/s. Due to previously explained conservatism, the outputs are being assessed against a threshold of sigma w being above or below 0.20 m/s.

The chart is somewhat 'busy' but can be interpreted as follows:

- the blue line is the measured sigma w values (corresponding with the left axis)
- the purple line is the ANN's estimated probability that sigma w is above or below 0.25 m/s (corresponding with the right axis)

- the black dotted line is the threshold value (0.2 m/s) and also 50% ANN-estimated probability
- the green/orange/red bar shows the model's output of 'safe', 'caution', or 'hazardous'; the occasional gaps are due to gaps in the source data
- the patchy bar of yellow and pink dots represent false alarms and misses, respectively. There are a few false alarms but very few misses (i.e. none in this example).

It can be seen that over this 48-hour period, the ANN successfully categorises a vast majority of all 10-minute time-steps. There are no periods where a hazardous condition is missed, but there are several 10-minute false alarm periods (almost all of which are due to the intentional conservativism). The 'caution' category aligns well with sigma w measurements nearing the threshold value. From a spray applicator's perspective, the output categories of safe/caution/hazardous are easy to manage.

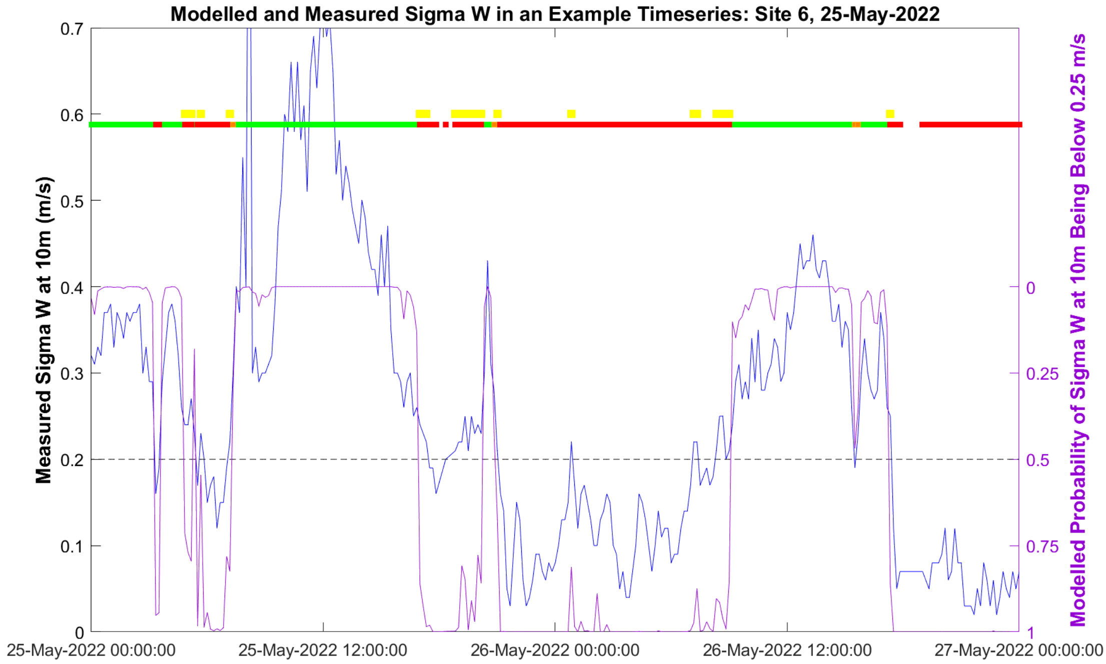

Figure 4. Example of the ANN estimating the real-time sigma w as above or below a 0.25m/s threshold

7. TWO-HOUR PREDICTION WINDOW FOR SIGMA W

Many farmers and spray applicators have expressed desire to have a forecast of whether there is likely to be a hazardous condition within the next 2-hours. This is because there is a significant set-up time involved before spraying begins, and they don't want to waste time setting up to then find that a hazardous condition has formed as soon as they're ready to spray. It also provides advance notice to begin finishing spray operations.

The ANN was tweaked to trial short-term future predictions. This was trialled for 1-hour, 2-hour and 3-hour predictions whereby the real-time value of sigma w was used within the ANN. A separate trial was done whereby the real-time value of sigma w was not used within the ANN.

The input data was prepared as described in previous sections, with the binary output representing either zero hazardous conditions in the 2-hour window, or, at least one timestep within the 2-hour window classified as hazardous conditions. As with the previous section, conservatism was introduced by using a sigma w threshold of 0.25 instead of 0.20 m/s. The same ANN was used as for Run D, E and F in Section 7.

7.1. Results and comparison

As expected, the success of the modelled predictions reduced as the length of the future prediction window increased (i.e. 3-hour prediction was less accurate than 1-hour prediction). The results are shown in Table 4.

Given that industry has requested a 2-hour prediction window, Run H was selected for those stations with real-time sigma w available. Interestingly, the success metrics for the prediction which does not use real-time sigma w (i.e. Run J) was only slightly worse than Run H. This is not unexpected given the success of the ANN in Section 6.1 which estimates real-time sigma w.

Conservative predictions of a 2-hour window with no hazardous conditions were correct 88% of the time with a Hit Rate of 93% and a False Alarm Rate of 16%. This level of accuracy is high enough such that this prediction would be considered useful to industry.

Table 4. ANN performance metrics for future predictions (based on threshold of sigma w = 0.25 m/s)

Run ID	Trial Run	CSI	Hit Rate	False Alarm Rate	Proportion Correct	Yule's Q
G	1-hr prediction: real-time sigma w	0.827	0.895	0.059	0.922	0.986
H	2-hr prediction: real-time sigma w	0.806	0.888	0.094	0.897	0.974
I	3-hr prediction: real-time sigma w	0.799	0.886	0.131	0.878	0.962
J	2-hr prediction: without real-time sigma w	0.802	0.885	0.097	0.895	0.973
K	2-hr prediction: real-time sigma w (assessment threshold sigma w = 0.2)*	0.788	0.930	0.159	0.885	0.990
L	2-hr prediction: without real-time sigma w (assessment threshold sigma w = 0.2)*	0.782	0.928	0.164	0.880	0.989

* Probabilities of 20% - 50% removed as 'caution'.

8. CONCLUSION AND RECOMMENDATIONS

A logistic artificial neural network (ANN) was used to optimise estimates for real-time sigma w being above or below a threshold value. Sigma w below the threshold value corresponds to hazardous spray conditions and represents a danger for long-distance spray drift to occur.

The resultant ANN performed very well with a Critical Success Index (CSI) of 0.997, a Hit Rate of 99%, a False Alarm rate of 9% and an overall 93% proportion correct. This compares favourably to a comparative check of the multivariate regression algorithm which used the Monin-Obukhov Stability Theory (Hit Rate of 81%), and compares very favourably to the current regulations which ban spraying during any inversion (i.e. False Alarm rate of 38%). In addition to the various performance metrics, an example 48-hour period chart shows the ANN has excellence performance.

A logistic ANN was also optimised for a 2-hour 'safe spray window' which can provide predictions for farmers for two hours into the future. A 2-hour safe spray window prediction is considered highly useful to spray applicators and growers for practicality reasons. It performed reasonably well with a Hit Rate of 93% and a False Alarm Rate of 16%.

These resultant real-time and predictive ANN algorithms can be used with the existing COtL Mesonet and would empower farmers with relevant real-time data. They can help to reduce the amount of pesticides in non-target areas while providing farmers with greater operational flexibility.

It is recommended that the ANNs be reviewed and retrained each year using a wider range of data, because ANNs are only useful over the range of inputs on which they were trained. Applying a more specialised machine learning expertise would likely yield some small improvements compared to this fairly basic ANN.

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