Selection of Independent Binary Features Using Probabilities: An Example from Veterinary Medicine

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We consider supervised classification into c mutually exclusive classes based on n binary features. The only information available is an $n \times c$ table with probabilities. Knowing that "the best d features are not the d best", we ran simulations for 4 feature selection methods and show an application to diagnosing BSE in cattle and Scrapie in sheep.

Keywords: Feature selection, classification, independent features, binary features, veterinary medicine.

Introduction

Consider the differential diagnosis of BSE in cattle based on the probabilistic description of BSE and 56 alternative diseases with similar symptoms. There are many possible disease-related signs that may be observed as present/absent on an animal. For example, we can list over 240 signs related to BSE and the 56 other diagnoses (Brightling et al. (1996), White (1984)). To build a diagnostic system, a data set is needed with observations for a number of cattle with their verified diagnoses. In the lack of such a data set, we rely on estimates of the individual class-conditional probabilities that sign x_i is present, given disease ω_i , where $i \in \{1, 2, ..., n\}$ and $j \in \{1, 2, ..., c\}$. information available in our problem is organized as shown in Table 1.

Table 1. Class-conditional probabilities for the individual features (the only information available)

	$\omega_{\rm l}$	$$ ω_i $$	ω_c
x_1			
		•••	
x_k		$P(x_k = 1 \mid \boldsymbol{\omega}_i)$	
\mathcal{X}_n		•••	

It is unrealistic to expect that a system based on these probabilities will fare well in practice because no relationship between the diagnostic signs (features) has been taken into account. In an ideal scenario, a data set will be collected using all features and the relationships between the features will be estimated from it. In reality, measuring only a small number of relevant features may be feasible.

We wish to select d features (d < n) which form a subset with the smallest classification error. Denote by \mathbf{x} the binary vector with the n features. The features are assumed to be conditionally independent, that is,

$$P(\mathbf{x} \mid \boldsymbol{\omega}_j) = \prod_{i=1}^n P(x_i \mid \boldsymbol{\omega}_j)$$
 (1)

The assumption of independence is enforced upon this study because only (some estimates of) the individual classconditional probabilities are available. Pattern recognition literature in the 1970s abounds with analyses of the case of independent binary features. Perhaps the most curious result is due to Toussaint (1971). If there are three independent binary features, the best combination of two features may not include the single best feature. Thus the most desirable selection criterion - the probability of error - will not guarantee the optimal solution if applied in a stepwise manner as in stepwise linear regression.

In this study we examine four procedures for selecting a subset of features and compare the results with those obtained with the whole feature set. We illustrate the feature selection methods on two problems taken from veterinary

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medicine: differential diagnosis of BSE in cattle and Scrapie in sheep.

Methods

Feature selection is one of the oldest topics in pattern recognition and machine learning (Stearns (1976), Van Campenhout (1982), Jain & Chandrasekaran (1982), Patrick (1972)). Surveys on more recent state-of-the-art and comparisons between feature selection procedures can be found in (Dash and Liu (1997), Blum and Langley (1997), Jain and Zongker (1997), Aha & Bankert (1995)).

Evaluation of the Feature Subsets

Because we are interested in the error of the classifier based on the feature subset, the most natural criterion would be the classification error. In theory we can calculate the error under the assumption that the probabilities are equal to their expert estimates. The optimal classifier for independent features is the Naïve Bayes classifier. Denote by P_j the prior probability for class ω_j . Let $\mathbf{x} = [x_1, ..., x_n]^T$ be a binary vector to be labeled into one of the c mutually exclusive classes. A discriminant function is calculated for each class.

$$\mu_{j}(\mathbf{x}) = P_{j}P(\mathbf{x} \mid \boldsymbol{\omega}_{j}) =$$

$$= P_{j} \prod_{i=1}^{n} P(x_{i} \mid \boldsymbol{\omega}_{j}), \quad j = 1,...,c$$
(2)

 \mathbf{x} is labeled in the class with the largest discriminant value. There are 2^d possible binary vectors \mathbf{x} for a candidate subset S with d features. The (probability for the) minimum classification error for the subset can be calculated as

$$P_{e} = \sum_{\mathbf{x}} P(\mathbf{x}, \text{error}) =$$

$$= 1 - \sum_{\mathbf{x}} \max_{j} \left[P_{j} \prod_{i \in S} P(x_{i} \mid \boldsymbol{\omega}_{j}) \right]$$
(3)

Equation (3) shows the difficulty in calculating the error for large d. We have to visit every \mathbf{x} and decide which class label to assign to it. There are indirect criteria related to the error which may be faster to calculate but direct calculation of

the error in some form is preferable (Dash & Liu (1997)). We chose to use Monte Carlo simulations for estimating the error of the selected feature subset. As we have the probabilities for each class, we generated randomly a sample from each class. Using the selected feature subset, we applied the Naïve Bayes classifier for the objects in this sample (supposedly a much smaller number than 2^d).

The Single-Best Method (SB)

It is known that the individually best d features do not necessarily form the best subset of d features (Toussaint (1971)). Nonetheless the method is quick and sometimes surprisingly efficient. We calculate the error for each feature separately using (3) (note that there are only two possible \mathbf{x} 's for each feature: present or absent), sort the errors in ascending order and retain the top d features. In this method we can pick a desired value for d.

The complexity of a feature selection algorithm is typically measured by the number of calculations of the classification error needed to select d out of n features. Thus the single-best method needs just n evaluations regardless of the number d.

Sequential Forward Selection (SFS)

This is the method traditionally used in stepwise regression. We start with an empty set, S, of chosen features, evaluate each feature separately as in the single-best method, and put the best individual feature in S. At the next step we evaluate all pairs of features which contain the feature selected already and one other feature. The pair with the smallest error is retained as S. Then we check all triples of features, and so on, until the desired cardinality d of S is reached. This procedure does not guarantee finding the optimal set of d features even in this simple case of independent binary features. The reason for this can be explained again with the Toussaint's counter example: the best set of two does not necessarily contain the single best feature.

Below we show an example illustrating both the non-optimality of the sequential feature selection (SFS) and the calculation of the error though equation (3).

Consider three features, x_1 , x_2 , and x_3 , and two classes, $\Omega = \{\omega_1, \omega_2\}$. The "non-traditional" data which we consider in this study is given in the form of probability estimates $P(x_i = 1 \mid \omega_j)$, as shown in Table 2.

Table 2. An example of a set of probabilities for 3 features and 2 classes

	ω_{l}	ω_2
x_1	0.1	0.5
x_2	0.6	0.1
x_3	0.8	0.4

Denote $a = P(x_k = 1 \mid \omega_1)$ and $b = P(x_k = 1 \mid \omega_2)$ for some x_k . Assuming equal prior probabilities for the two classes, the probability of correct classification for feature x_k is

$$P(k) = 1/2 \{ \max(a,b) + \max(1-a,1-b) \}$$
(4)

Using (4), the individual errors for the

features are $\varepsilon_1 = 1 - \frac{1}{2} [\max(.1,.5) + \max(.9,.5)] = 0.30$, $\varepsilon_2 = 0.25$, and $\varepsilon_2 = 0.30$. Consider a pair of features, (x_k, x_j) , and denote the probabilities for x_j as $p = P(x_j = 1 \mid \omega_1)$ and $q = P(x_j = 1 \mid \omega_2)$. Substituting again in eqn (3), the probability of correct classification for the pair of features is

$$P(k, j) = 1/2 \{ \max(ap, bq)$$

$$+ \max[(1-a)p, (1-b)q]$$

$$+ \max[a(1-p), b(1-q)]$$

$$+ \max[(1-a)(1-p), (1-b)(1-q)] \}$$
(5)

The errors for the three pairs of features for the example in Table 2 are $\mathcal{E}_{12} = 1 - \frac{1}{2} (\max(.1 \times .6, .5 \times .1))$

$$+ \max(.9 \times .6, .5 \times .1)$$

+
$$max(.1x.4,.5x.9)$$

+
$$max(.9 \times .4,.5 \times .9)$$
)
= 0.25,

 $\varepsilon_{13} = 0.24$, and $\varepsilon_{23} = 0.25$.

As ε_{13} is the smallest pair-wise error, and ε_2 is the smallest individual error, the best pair of independent features, (x_1,x_3) , does not include the single best feature x_2 .

SFS is probably the most widely used procedure because it has both reasonable error and reasonable complexity for "traditional" data sets (Aha & Bankert (1995), Jain & Zongker (1997)).

At the first step SFS evaluates all n features, at the second step, n-1 evaluations are needed as there are n-1 possible pairs. For selecting d features, SFS needs the following number of evaluations of the error

$$\sum_{i=0}^{d-1} (n-i)$$
 (5)

However, the complexity calculation is not that simple when we select the features from probabilistic data as shown in Table 1. For the calculation of the theoretical error the algorithm has to visit every \mathbf{x} in the possible feature space, find out which the maximum discriminant function is, and add the contribution of the error for \mathbf{x} based on the class label decision. The fact that the features are treated as independent does not make the task any easier. The complexity of SFS will depend heavily on the number of features in the evaluated subsets.

Complexity of feature selection algorithms for probabilistic data can be evaluated by the total number of \mathbf{x} 's visited in the process of selecting d out of the n features. The complexity for the single-best method is $C_{SB} = 2n$., and for the SFS, $C_{SFS} = \sum_{i=0}^{d-1} (n-i)2^{i+1}$.

Class-Pairs Feature Selection (CP)

Ji & Bang (2000) propose the following feature selection method. A single feature is selected for each pair of classes.

Table 3 shows the data structure used by the algorithm, where C_{ij} = class pairs, ($i \neq j$), $x_k = k$ -th feature, (k = 1,...,n), $P_{ij}(k)$ = discriminatory power of feature k for C_{ij} . Using (4), we calculate the values of $P_{ij}(k)$ as the probability of correct

classification between classes ω_i and ω_j for feature x_k .

Table 3. The table for the class-pairs method for feature selection (Ji & Bang (2000))

	C_{ij}	
x_k	$P_{ij}(k)$	T_k
	E_{ij}	

We then calculate two vectors

- $E_{ij} = \sum_{k} P_{ij}(k)$, the relative ease of classifying the pair C_{ij} , and
- $T_k = \sum_{ij} P_{ij}(k)$, the relative discriminatory power of feature x_k .

We start with an empty set of features. The class pair that is the hardest to discriminate (has the smallest E_{ij}) is identified from the table. The feature with the highest discriminatory power for this pair is added to the subset, if not already selected. If more than one feature has the highest $P_{ii}(k)$ in the chosen column then we select the feature with the highest value of T_k . The "hardest" pair is removed from the table and the process continues with the next hardest pair of classes. (Note that the classes are not removed altogether, only the column of the table is removed.) We stop when al class pairs have been covered.

The maximum number of features this method will select is $\max\{(c(c-1)/2, n)\}$. However, Ji & Bang claim that the number selected will be much less than either of these. We may also restrict this method at any point to pick only d features. The complexity of the class-pair method (measured again by the total number of \mathbf{x} 's visited) is $C_{CP} = c$ (c-1) n. This calculation reflects only the preparation phase (setting up Table 3), and does not take into account the actual procedure which constructs the feature subset.

Feature-Pairs Feature Selection (FP)

The selection methods considered above are either overly simplistic but scale

well with *n*, *c*, and *d* (single-best) or computationally demanding but more accurate (SFS). Optimality of the selected feature subset is not guaranteed in any case. The class-pairs method is one possible method that scales well and may be accurate. Here we propose another method for feature selection from probabilities, called feature-pairs method.

We start with an empty set of features. All pairs of features are evaluated and the best pair is added to the set. While the desired number of features is not reached, add the features from the next best pair which are not already among the selected features. Suppose that d-1features are already in the set, and there is a pair of features such that neither of the two members of the pair is in the set. We may either take both features and exit with d+1 features or randomly select one member of the pair to make up the total of d features in the set. The complexity of the feature-pairs method (using the number of visited **x**'s) is $C_{FP} = n (n-1)$.

All four methods are based on a true calculation of the classification error plus some heuristic about how we form the feature subset. The experimental results in the next section help us evaluate the assets and drawbacks of the four methods.

Experiments and results

A Small-Scale Simulation Study

To include SFS in the comparisons, we started with a relatively small example with n = 20 features and varied the number of classes, c, from 3 to 10. The number of selected features, d, was varied from 2 to 10.

For each c, 50 random matrices of size $20 \times c$ were generated from uniform random distribution. Each matrix represented the probabilities for the features and classes as shown in Table 1. For each such matrix and each d, we applied the four feature selection algorithms and found the best subset of size d using the probabilities.

To evaluate the selected subsets, a "traditional" data set was generated randomly for every pair (c,d). One hundred data points were generated from

the distribution of each class and the Naïve Bayes classifier was used to label these points. The error was estimated as the percent mismatch with the true class label.

An example of the simulation algorithm is given below. Consider the problem presented in Table 2. Suppose that Method X picked features (x_1,x_3) . Set a misclassification counter to 0. The steps below are repeated 100 times for each class.

(Step 1) Generate a data point from class ω_1 . To do this, pick a vector of 3 random numbers, one for each features, e.g. $[0.2736, 0.9241, 0.7102]^T$. Compare it with the first column of Table 2 (corresponding to ω_1). If the generated number for x_i is smaller than the corresponding probability in the table, set x_i to 1, else set x_i to 0. For this example, the generated data point is $\mathbf{x} = [0,0,1]$.

(Step 2) Classify the data point using Naïve Bayes and only the chosen features. For this example, the two discriminant functions for **x** are

$$\mu_1(\mathbf{x}) = 1/2(0.9 \times 0.8) = 0.36$$

 $\mu_2(\mathbf{x}) = 1/2(0.5 \times 0.4) = 0.10$

(Step 3) Choose a class label by the maximum discriminant function and note whether there is a mismatch with the class label whose distribution we are currently using. In the example, label ω_1 is chosen so the misclassification counter remains unchanged.

Figure 1 shows the probability of error versus the number of selected features, d, for c = 10 classes. Each point on the figure is the average error over the 50 random matrices.

As expected, SFS gives the lowest error. The single-best and the feature-pairs methods are approximately the same with a slight preference to feature-pairs, and the class-pairs method is the worst. For d=2 selected features, SFS is the second best method because feature pairs selects the true best pair features.

Table 4 gives the classification error averaged across the 50 random matrices of probabilities for 2 and 10

selected features (out of 20), for c = 3,..., 10 classes.

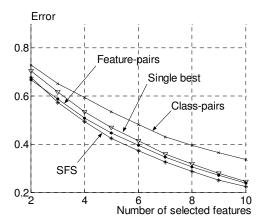


Figure 1. Probability of error versus the number of selected features (n=20, c=10).

Table 4. Classification error (in %) with 2 and 10 features for c = 3,..., 10 classes. CP stands for class-pairs method, SB for the single-best method and FP for the feature-pairs method.

(a)

(1-)

(a)				
	d = 2	selected t	features	
c	CP	SFS	SB	FP
3	21.2	17.9	22.7	16.8
4	40.1	31.7	36.1	30.3
5	49.6	42.9	47.2	41.1
6	57.9	51.0	54.2	49.4
7	62.6	56.2	60.3	54.3
8	67.5	61.3	64.3	59.4
9	70.2	65.1	67.8	63.8
10	72.8	67.8	70.6	66.8

(b)				
d = 10 selected features				
c	CP	SFS	SB	FP
3	14.4	4.2	4.4	4.5
4	16.8	7.3	7.9	8.0
5	16.1	9.8	10.8	11.2
6	21.2	13.7	15.0	15.1
7	25.0	15.5	17.2	17.3
8	29.1	18.4	20.4	19.8
9	31.2	20.8	23.0	22.8
10	33.6	22.3	24.3	23.9

The results in Table 4 confirm the superiority of SFS for more than 2 features and also shows that the class-pairs method gives the largest error. There is an interesting turn about the single-best and

feature-pairs methods. For small number of classes (3 to 7) SB was slightly better whereas for larger number of classes (8 to 10) FP was the better of the two methods. This behaviour is an indication that for larger scale problems FP may be the more accurate method.

A Larger-Scale Simulation Study

We excluded SFS from this experiment because of its large computational time. The same experiments as in the previous section were run with a total number of features n = 100 and number of classes c = 50. The number of selected features was $d \in \{5, 10, 15, ..., 50\}$. Figure 2 shows the error versus the number of selected features for SB, CP and FP.

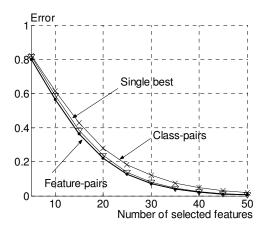


Figure 2. Probability of error versus the number of selected features (n = 100, c = 50).

The curves are close together but the errors for all d are related as $E_{\rm FP} < E_{\rm SB}$ $< E_{\rm CP}$. The differences between $E_{\rm FP}$ and $E_{\rm SB}$ are not statistically significant. Figure 3 shows the histogram of the 50 differences $E_{\rm SB}$ – $E_{\rm FP}$ for 50 and 25 selected features.

For 50 features, $E_{\rm SB} - E_{\rm FP}$ was positive in 64% of the runs, the same in 6% of the runs and negative in 30% of the runs. For 25 selected features, $E_{\rm SB} - E_{\rm FP}$ was positive in 94% of the runs and negative in 6% of the runs. This suggests that there may be optimal ratios c:d:n for which FP is distinctly better than SB.

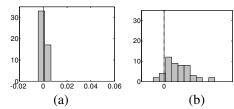


Figure 3. Histograms of the 50 differences $E_{SB} - E_{FP}$ for d = 50 selected features (a) and d = 25 selected features (b).

The computational time ratio for the three methods was approximately $C_{\rm SB}$: $C_{\rm CP}$: $C_{\rm FP}$ = 1:8:23.

The above simulations do not assume any relationship between the classes. The matrices are generated uniformly which means that the correlations between the columns will be close to 0 as will be the correlations between the rows. In real problems the class profiles will rarely be uncorrelated. Below we explore the four methods on two real diagnostic problems where only probabilistic data is available.

An Application to Diagnosis of BSE in cattle and Scrapie in Sheep

The above feature selection methods were applied for selecting diagnostic signs in two problems coming from veterinary medicine.

BSE and Scrapie are fatal neurodegene-rative diseases. Both are notifiable diseases which have no known cure. There is currently no ante-mortem test for the diseases that can be used routinely in the field. Notifiable diseases have a major impact on human health. welfare and economics. There was a BSE epidemic in Britain in the 90's and with the first ever BSE case diagnosed in the USA at the end of 2003, the problem of these diseases is global. Therefore, the recognition of the clinical presentations of the two diseases and the need to differentiate them from other diseases is important. In veterinary medicine prevalences of disease, the conditional dependencies of clinical signs and the sign frequencies within diseases are rarely, if ever available; demonstrating the need to work with probability data.

Table 5 shows the results from the feature selection experiments with the BSE data. We applied SFS to select 10 of the 242 features and simulated data from the distributions of the 57 classes. To find out how far the lower complexity methods are from SFS we ran SB, CP and FP for d = 10 features too. The first 4 rows in Table 4 show the classification error for d = 10 (as shown in the brackets).

Table 4. Results from feature selection on the BSE probabilities.

Method (d)	Error
SFS (10)	0.4258
SB (10)	0.6432
CP (10)	0.5865
FP (10)	0.5482
CP (58)	0.0172
SB (58)	0.0309
FP (58)	0.0256
ALL (242)	0.0049

Next we ran the class-pairs method letting it stop when all class pairs have been accounted for. CP selected a total of 58 features. Leaving SFS aside, we ran the other two low-complexity methods for 58 features. The classification error is displayed in rows 5-8 in Table 4. Finally, the error with using all features was estimated as a tight lower bound on the classification error.

The results show that the closest rival to SFS for small number of features is the FP method proposed here. Contrary to the results in the previous section though, CP is better than SB. This shows that in real-life problems when there is dependency between the classes, CP may be a better solution than SB. When run "all the way", CP provides the smallest classification error of the three low complexity methods followed by FP and then SB.

Note the large differences between the error probabilities for small number of features. These differences strongly suggest that SFS should be applied as long as the computation time is acceptable. To illustrate the differences between the selected sets of features, Table 5 shows the signs selected by SFS (a) and SB (b) in the order they entered the set.

The same pattern of experiments was repeated for the data containing the probabilities for Scrapie and 62 alternative diseases.

Table 5. Signs selected by SFS and SB for diagnosing BSE and 56 other diseases in cattle

(a) Signs selected by SFS

Gait abnormal, unspecified
Circling in one direction
Hypo-responsive to external stimuli
Milk yield less than normal (individual)
Rumen rate nil, (0 per 2min)
Eye menace response absent
Hyper-responsive to external stimuli
Dyspoena, unspecified
Posture recumbency
Temperature > 39.5 degrees Celsius

(b) Signs selected by SB

Gait abnormal, unspecified
Dyspoena, unspecified
Dyspoena, rate increased shallow
Diarrhoea, unspecified
Gait uncoordinated\exaggerated
Rumen rate slow (1 per 2min)
Diarrhoea, acute, profuse
Circling in one direction
Gait stiff
Head rotated, tilted or deviated

Twelve features were selected by SFS. We run the 3 lower-complexity methods for d = 12. The errors are shown in Table 6.

Table 6. Results from feature selection on the Scrapie probabilities.

Method (<i>d</i>)	Error
SFS (12)	0.5975
SB (12)	0.7635
CP (12)	0.6930
FP (12)	0.6610
CP (77)	0.0625
SB (77)	0.0992
FP (77)	0.0649
ALL (285)	0.0252

The class-pairs method (CP) was run again until all class pairs were covered. The

number of selected features was 77. SB and FP were then run for the same number of features. Table 6 ranks the feature selection methods exactly in the same way as Table 4. Again, the discrepancies with our simulation study in the previous subsection can be attributed to the fact that the classes here are not independent. The CP method manages to capture some dependency between the classes and, if run "all the way", it selects better subsets of features than SB and FP. Table 7 mirrors table 5 by showing the signs selected for diagnosing Scrapie and the 63 alternative diseases.

Table 7. Signs selected by SFS and SB for diagnosing Scrapie and 63 other diseases in sheep

(a) Signs selected by SFS

Foul odour skin

Mastitis

Exercise intolerance

Paraparesis

Weight Loss

Generalized weakness

Anorexia

Generalized lameness or stiffness

Ataxia

Underweight, thin etc

Dullness

Reluctant to move

(b) Signs selected by SB

Foul odour skin

Mastitis

Matted \ dirty wool \ hair

Moist skin\wool \hair

Skin necrosis

Exercise intolerance

Hyperkeratosis

Lymphadenopathy

Alopecia

Pruritus

Weight loss

Dullness

Conclusions

We explore the problem of selecting a subset of n binary features to discriminate between c mutually exclusive classes. We assume that we do not have a "traditional" data set containing the description of a set

of objects with known class labels. The information available here is in the form of an $n \times c$ table with class-conditional probabilities for the binary features, i.e., $P(x_i=1|\omega_i), i = 1,...,n, j = 1,...,c.$ No relationship between the features is assumed. Selecting the best subset of features seems easy because all the information probabilistic (plus assumption of independence) is available. In practice, however, the problem is not as simple. It is known that the individually best d features do not necessarily form the best subset of d features. This leads to the need to check many subsets - the more, the better. The second obstacle is the calculation of the theoretical error for a given subset. An easy way out would be to generate a sample and run it through the Naïve Bayes classifier using only the features in the subset. We applied three methods from the literature (SFS, SB and CP) and proposed a method based on features pairs (FP) for feature selection using probabilities. Our study showed that SFS was the most accurate and the most computationally demanding of the four methods. The simulation experiments with random generated matrices with probabilities suggested that CP was inferior to SB and FP but did not favour strongly any of the two. The experiments with two real data matrices from veterinary medicine demonstrated that CP is also a valuable method when larger subsets of features are acceptable. FP was found to be the best alternative to SFS for small and medium subsets.

There are at least two caveats which we are aware of. First, features are rarely independent in real life problems. By assuming independence, we do run the risk of missing an important feature which does not have a reasonable predictive value on its own but is highly important in combination with others. However, in the absence of any further information, the independence assumption is the only option. Second, the estimates of the probabilities given as the information to work upon (Table 1) might not be very close to the true probabilities. A sensitivity study can be run by perturbing the probability estimates and observing how the selected feature subset changes.

The acid test for the quality of the selected subset of features would be the error on real data. However, our aim here is a preliminary feature selection so that a real data set can be collected using these features. Therefore, at this stage we should provide a "reasonably" large feature set. The hope is that it will contain highly discriminative combinations of features which will be discovered later using the collected data.

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