Supplementary material:
Efficient Feature Selection Using Shrinkage Estimators

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A Proof of Theorems

A.1 Proof of Theorem 1

For this proof we will use Ledoit and Wolf theorem (Ledoit and Wolf, 2003), which derives an analytical expression for the optimal shrinkage intensity that guarantees minimal MSE. Using the fact that $\hat{p}_{\text{ML}}(xy)$ is an unbiased estimator of $p(xy)$, the optimal shrinkage intensity takes the following form (Hausser and Strimmer, 2009, eq. (10)):

$$
\lambda^* = \frac{\sum_{x \in X} \sum_{y \in Y} \left( \text{Var} \left[ \hat{p}_{\text{ML}}(xy) \right] - \text{Cov} \left[ \hat{p}_{\text{ML}}(xy), \hat{p}_{\text{Ind}}(xy) \right] \right)}{\sum_{x \in X} \sum_{y \in Y} \left( E \left[ \left( \hat{p}_{\text{ML}}(xy) \right)^2 \right] + E \left[ \left( \hat{p}_{\text{Ind}}(xy) \right)^2 \right] - 2 E \left[ \hat{p}_{\text{ML}}(xy) \hat{p}_{\text{Ind}}(xy) \right] \right)}
$$

Following Hausser and Strimmer (2009) approach, we can derive a simple estimate of $\lambda^*$ by replacing all variances, covariances and expectations with their empirical counterparts (Schäfer and Strimmer, 2005, eq. (8)):

$$
\hat{\lambda}^* = \frac{\sum_{x \in X} \sum_{y \in Y} \left( \text{Var} \left[ \hat{p}_{\text{ML}}(xy) \right] - \text{Cov} \left[ \hat{p}_{\text{ML}}(xy), \hat{p}_{\text{Ind}}(xy) \right] \right)}{\sum_{x \in X} \sum_{y \in Y} \left( E \left[ \left( \hat{p}_{\text{ML}}(xy) \right)^2 \right] + E \left[ \left( \hat{p}_{\text{Ind}}(xy) \right)^2 \right] - 2 E \left[ \hat{p}_{\text{ML}}(xy) \hat{p}_{\text{Ind}}(xy) \right] \right)}
$$

To derive the expressions of the five terms we will assume a random vector $N$, whose elements are the counts $N_{xy}$, which is distributed as a $|X||Y|$ Multinomial random variable. The parameters are $N$, the total number of observations, and $p$, the vector of the true underlying probabilities $p(xy)$. Under this assumption we will derive estimates for the five terms of eq. (1).
• **First term:** The first term can be written as follows:

\[
\text{Var} \left[ \hat{p}^{\text{ML}}(xy) \right] = \text{Var} \left[ \frac{N_{xy}}{N} \right] = \frac{1}{N^2} \left( E \left[ N_{xy}^2 \right] - E \left[ N_{xy} \right]^2 \right) \tag{2}
\]

Under the Multinomial modelling, the first two moments are (Mosimann, 1962):

\[
E \left[ N_{xy} \right] = Np(xy) \tag{3}
\]

\[
E \left[ N_{xy}^2 \right] = N(N - 1)p(xy)^2 + Np(xy) \tag{4}
\]

By substituting eqs (3) and (4) into eq. (2) we get:

\[
\text{Var} \left[ \hat{p}^{\text{ML}}(xy) \right] = \frac{1}{N^2} \left( N(N - 1)p(xy)^2 + Np(xy) - N^2p(xy)^2 \right) = \frac{p(xy)}{N}(1 - p(xy))
\]

The above term can be estimated as

\[
\bar{\text{Var}} \left[ \hat{p}^{\text{ML}}(xy) \right] = \frac{\hat{p}^{\text{ML}}(xy)}{N} \left( 1 - \hat{p}^{\text{ML}}(xy) \right)
\]

• **Second term:** The covariance term can be written as follows:

\[
\text{Cov} \left[ \hat{p}^{\text{ML}}(xy), \hat{p}^{\text{Ind}}(xy) \right] = E \left[ \hat{p}^{\text{ML}}(xy) \hat{p}^{\text{Ind}}(xy) \right] - E \left[ \hat{p}^{\text{ML}}(xy) \right] E \left[ \hat{p}^{\text{Ind}}(xy) \right]
\]

\[
= \frac{1}{N^3} \left( E \left[ N_{xy}N_yN_{y'} \right] - E \left[ N_{xy} \right] E \left[ N_{y}N_{y'} \right] \right) \tag{5}
\]

The expected value \(E[N_xN_y]\) can be calculated as follows:

\[
E \left[ N_xN_y \right] = \sum_{x' \in X} \sum_{y' \in Y} \sum_{x' \neq x} \sum_{y' \neq y} E \left[ N_{xy'}N_{x'y'} \right] + \sum_{x' \neq x} \sum_{y' \neq y} E \left[ N_{xy}N_{x'y'} \right] + E \left[ N_{xy}^2 \right] \tag{6}
\]

Under the Multinomial modelling, the second order moments can be written as follows (Mosimann, 1962):

\[
E \left[ N_{xy}N_{x'y'} \right] = N(N - 1)p(xy)p(x'y') \tag{7}
\]

\[
E \left[ N_{xy}N_{x'y'} \right] = N(N - 1)p(xy)p(x'y') \tag{8}
\]

By substituting eqs (4),(7) and (8) into eq. (6) we get:

\[
E \left[ N_xN_y \right] = N(N - 1) \left( \sum_{x' \in X} \sum_{y' \in Y} p(xy)p(x'y') + \sum_{x' \in X} p(xy)p(x'y') + p(xy)^2 \right) + Np(xy)
\]

\[
= N(N - 1) \left( \sum_{y' \in Y} p(xy)p(y) + \sum_{x' \in X} p(xy)p(x'y') + p(xy)^2 \right) + Np(xy)
\]

\[
= N(N - 1) \left( p(x) - p(xy) \right) p(y) + p(xy) \left( p(y) - p(xy) \right) + p(xy)^2 \right) + Np(xy)
\]

By simple computation, we obtain

\[
E \left[ N_xN_y \right] = N(N - 1)p(x)p(y) + Np(xy) \tag{9}
\]

Now we will calculate the expected value \(E[N_{xy}N_xN_y]\). This expectation can be written as follows:

\[
E \left[ N_{xy}N_xN_y \right] = \sum_{x' \in X} \sum_{y' \in Y} E \left[ N_{xy'}N_{x'y'}N_{x'y'} \right]
\]
The above term can be estimated as

\[
\sum_{x' \in X} \sum_{y' \in Y} E[N_{xy} N_{x'y'}] + \sum_{x' \in X} E[N_{xy}^2 N_{x'y'}] + \sum_{y' \in Y} E[N_{xy}^2 N_{x'y'}] + E[N_{xy}^3]
\]

By simple computation, we obtain

Under the Multinomial modelling, the third order moments can be written as follows (Mosh-mann, 1962):

\[
E[N_{xy} N_{x'y'}] = N(3)p(xy)p(xy')p(x'y) 
\]

\[
E[N_{xy}^2 N_{x'y'}] = N(3)p(xy)^2 p(x'y) + N(2)p(xy)p(x'y)  
\]

\[
E[N_{xy}^2 N_{x'y'}] = N(3)p(xy)^2 p(xy') + N(2)p(xy)p(x'y) 
\]

\[
E[N_{xy}^3] = N(3)p(xy)^3 + 3N(2)p(xy)^2 + Np(xy) 
\]

where \(N(2) = N(N - 1)\) and \(N(0) = N(N - 1) \cdots (N - a + 1)\), for a > 2.

By substituting eqs (11) - (14) into eq. (10), we get:

\[
E[N_{xy} N_{x'y'}] = \sum_{x' \in X} \sum_{y' \in Y} N(3)p(xy)p(xy')p(x'y) 
\]

\[
+ \sum_{x' \in X} N(3)p(xy)^2 p(x'y) + N(2)p(xy)p(x'y)  
\]

\[
+ \sum_{y' \in Y} N(3)p(xy)^2 p(xy') + N(2)p(xy)p(x'y) 
\]

\[
+ N(3)p(xy)^3 + 3N(2)p(xy)^2 + Np(xy) \Rightarrow 
\]

\[
E[N_{xy} N_{x'y'}] = N(3)p(xy)(p(x) - p(xy))(p(y) - p(xy)) 
\]

\[
+ N(3)p(xy)^2 (p(y) - p(xy)) + N(2)p(xy)(p(y) - p(xy)) 
\]

\[
+ N(3)p(xy)^2 (p(x) - p(xy)) + N(2)p(xy)(p(x) - p(xy)) 
\]

\[
+ N(3)p(xy)^3 + 3N(2)p(xy)^2 + Np(xy) 
\]

By simple computation, we obtain

\[
E[N_{xy} N_{x'y'}] = N(3)p(xy)p(xy')p(x'y) + N(N - 1)p(xy)p(y) + Np(xy)  
\]

Thus, by substituting eqs (3), (9) and (15) into eq. (5), we get:

\[
\text{Cov}\left[\hat{p}_{\text{ML}}(xy), \hat{p}_{\text{Ind}}(xy)\right] = \frac{1}{N^2} \left[ N(3)p(xy)p(xy) + N(N - 1)p(xy)p(y) + Np(xy) 
\]

\[
- \left( N(N - 1)p(xy) + Np(xy) \right) 
\]

Again, by simple computation, we obtain:

\[
\text{Cov}\left[\hat{p}_{\text{ML}}(xy), \hat{p}_{\text{Ind}}(xy)\right] = \frac{p(xy)}{N^2} \left( (N - 1)(p(x) + p(y) - 2p(xy)) + 1 - p(xy) \right) 
\]

The above term can be estimated as

\[
\text{Cov}\left[\hat{p}_{\text{ML}}(xy), \hat{p}_{\text{Ind}}(xy)\right] = \frac{\hat{p}_{\text{ML}}(xy)}{N^2} \left( (N - 1)(\hat{p}_{\text{ML}}(x) + \hat{p}_{\text{ML}}(y) - 2\hat{p}_{\text{ML}}(x)\hat{p}_{\text{ML}}(y)) + 1 - \hat{p}_{\text{ML}}(xy) \right) 
\]
Finally, the above term can be estimated as
\[
\mathbb{E} \left( \left( \hat{p}_{ML}^{xy} \right)^2 \right) = \frac{p(xy)}{N} \left( (N - 1)p(xy) + 1 \right)
\]

Using eq. (4), the last expression can be written as
\[
\mathbb{E} \left( \left( \hat{p}_{ML}^{xy} \right)^2 \right) = \frac{p(xy)}{N} ((N - 1) \hat{p}_{ML}^{xy} + 1)
\]

According to the known fourth order moments formulas (Mosimann, 1962), we need to treat the terms in eq. (16) by splitting them into five categories:
A. four different terms;
B. three different terms over four;
C. two different terms over four (two couples equal);
D. two different terms over four (a triplet and a single element);
E. a single element to the power four.

The sum of fourth order moments can thus be written as the sum of five different terms, i.e.,
\[
\sum_{x',z'' \in X} \sum_{y',y'' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x''y''}N_{x'y''}N_{x''y'} \right] = A(xy) + B(xy) + C(xy) + D(xy) + E(xy),
\]

where
\[
A(xy) = \sum_{x',z'' \in X} \sum_{y',y'' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x''y''}N_{x'y''}N_{x''y'} \right] + 2 \sum_{x' \in X} \sum_{y',y'' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x'y''}N_{x'y''}N_{x'y} \right],
\]
\[
B(xy) = \sum_{x',z'' \in X} \sum_{y' \in Y} \mathbb{E} \left[ N_{x'y}N_{x'y''}N_{x'y''}N_{x'y} \right] + 2 \sum_{x' \in X} \sum_{y'' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x'y}N_{x'y''}N_{x'y} \right]
\]
\[
+ \sum_{x' \in X} \sum_{y',y'' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x'y}N_{x'y''}N_{x'y''} \right] + 2 \sum_{x' \in X} \sum_{y' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x'y}N_{x'y}N_{x'y''} \right]
\]
\[
+ 4 \sum_{x' \in X} \sum_{y',y'' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x'y''}N_{x'y'}N_{x'y''} \right],
\]
\[
C(xy) = \sum_{x' \in X} \sum_{y' \in Y} \mathbb{E} \left[ N_{x'y'}N_{x'y'}N_{x'y'}N_{x'y'} \right] + \sum_{x' \in X} \mathbb{E} \left[ N^2_{x'y'}N_{x'y'} \right],
\]
\[
D(xy) = 2 \sum_{x' \in X} \sum_{y' \in Y} \mathbb{E} \left[ N^3_{x'y'}N_{x'y'} \right] + 2 \sum_{y' \in Y} \mathbb{E} \left[ N^3_{x'y'}N_{x'y'} \right],
\]
\[
E(xy) = \sum_{x' \in X} \sum_{y' \in Y} \mathbb{E} \left[ N^4_{x'y'}N_{x'y'} \right].
\]
Under the Multinomial modelling, the fourth order moments that we need to calculate these five terms can be written as follows (Mosimann, 1962):

(Eq. 17) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)p(xy)p(x'y)p(x''y))
\]

(Eq. 18) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)p(xy)p(x'y)p(xy))
\]

(Eq. 19) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)p(x'y)p(x''y)p(x''y)) + N^3 (p(xy)p(x'y)p(x''y)p(xy))
\]

(Eq. 20) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)p(xy)p(x'y)^2 + N^3 (p(xy)p(xy)p(x''))p(xy)
\]

(Eq. 21) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)p(xy)p(x'y)^2 + N^3 (p(xy)p(xy)p(xy)p(x''))p(xy)
\]

(Eq. 22) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)p(xy)p(x'y)^2 + N^3 (p(xy)p(xy)p(xy)p(x'))p(xy)
\]

(Eq. 23) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)^2 + N^3 (p(xy)p(x'y) (p(xy) + p(x'')) + N^2 (p(xy)p(x'))
\]

(Eq. 24) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)^2 + N^3 (p(xy)p(x'y) (p(xy) + p(x'')) + N^2 (p(xy)p(x'))
\]

(Eq. 25) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)^2 + N^3 (p(xy)p(x'y) (p(xy) + p(x'')) + N^2 (p(xy)p(x'))
\]

(Eq. 26) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)^2 + N^3 (p(xy)p(x'y) (p(xy) + p(x'')) + N^2 (p(xy)p(x'))
\]

(Eq. 27) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)^2 + N^3 (p(xy)p(x'y) (p(xy) + p(x'')) + N^2 (p(xy)p(x'))
\]

(Eq. 28) \[
\mathbb{E} \left[ N_{xy} N_{x'y} N_{x''y} N_{x'''y} \right] = N^4 (p(xy)^2 + N^3 (p(xy)p(x'y) (p(xy) + p(x'')) + N^2 (p(xy)p(x'))
\]

Using eqs (17) - (28) and some simple computation, we obtain the following expressions for the five terms:

\[
A(xy) = N^4 \left[ \left( p(x)^2 - \sum_{y' \in \mathcal{Y}} p(xy')^2 \right) \left( p(y)^2 - \sum_{x' \in \mathcal{X}} p(x' y)^2 \right) \right.
\]

\[
B(xy) = N^4 \left[ \sum_{y' \in \mathcal{Y}} p(xy')^2 \left( p(y)^2 - \sum_{x' \in \mathcal{X}} p(x' y)^2 \right) - 2p(xy)^3 (p(y) - p(xy)) \right.
\]

\[
C(xy) + D(xy) = N^4 \left[ \sum_{x' \in \mathcal{X}} p(x' y)^2 \sum_{y' \in \mathcal{Y}} p(xy')^2 \right.
\]

\[
+ N^3 \left[ 4p(xy)^3 + p(x) \sum_{x' \in \mathcal{X}} p(x' y)^2 + p(y) \sum_{y' \in \mathcal{Y}} p(xy')^2 \right]
\]
\[D(xy) = 2N^{(4)} \left[ p(xy)^3 (p(x) + p(y) - 2p(xy)) \right] + 6N^{(3)} p(xy)^2 (p(x) + p(y) - 2p(xy)) + 2N^{(2)} p(xy) (p(x) + p(y) - 2p(xy)).\]

By simple computation, we obtain
\[\sum_{x', y', x'' \in X, y', y'' \in Y} E \left[ N_{xy'} N_{xy''} N_{x'y'} N_{x''y''} \right] = N^{(4)} p(x)^2 p(y)^2 + N^{(3)} p(x)p(y)(p(x) + p(y) + 4p(xy)) + N^{(2)} \left[ 2p(xy)(p(x) + p(y)) + 2p(xy)^2 + p(x)p(y) \right] + N p(xy).\]

Since the parameters \(p(xy)\) are unknown, we substitute the ML estimates in order to estimate the second moment of \(\hat{p}^{\text{Ind}}(xy)\), i.e.,
\[
\hat{E} \left[ (\hat{p}^{\text{Ind}}(xy))^2 \right] = \frac{1}{N} \left( (N - 1)(N - 2)(N - 3) \left( \hat{p}^{\text{ML}}(x) \hat{p}^{\text{ML}}(y) \right)^2 + (N - 1)(N - 2)\hat{p}^{\text{ML}}(x) \hat{p}^{\text{ML}}(y) \left( \hat{p}^{\text{ML}}(x) \hat{p}^{\text{ML}}(y) + 4\hat{p}^{\text{ML}}(xy) \right) \right) + \left( N - 1 \right) \left( 2\hat{p}^{\text{ML}}(xy) \hat{p}^{\text{ML}}(x) \hat{p}^{\text{ML}}(y) + 2\hat{p}^{\text{ML}}(xy) \hat{p}^{\text{ML}}(x) \hat{p}^{\text{ML}}(y) + \hat{p}^{\text{ML}}(xy) \right) \right).
\]

**Fifth term:** This expectation term can be calculated as follows:
\[E \left[ \hat{p}^{\text{ML}}(xy) \hat{p}^{\text{Ind}}(xy) \right] = \frac{1}{N^2} E \left[ N_{xy} N_{xy} \right] \]

Using eq. (15), the last expression can be written as
\[E \left[ \hat{p}^{\text{ML}}(xy) \hat{p}^{\text{Ind}}(xy) \right] = \frac{p(xy)}{N^2} \left( (N - 1)(N - 2)p(x)p(y) + (N - 1)(p(y) + p(x) + p(xy)) + 1 \right) \]

Finally, the above term can be estimated as
\[
\hat{E} \left[ \hat{p}^{\text{ML}}(xy) \hat{p}^{\text{Ind}}(xy) \right] = \frac{\hat{p}^{\text{ML}}(xy)}{N^2} \left( (N - 1)(N - 2)\hat{p}^{\text{ML}}(x) \hat{p}^{\text{ML}}(y) + (N - 1) \left( \hat{p}^{\text{ML}}(x) \hat{p}^{\text{ML}}(y) + \hat{p}^{\text{ML}}(xy) \right) + 1 \right)
\]

A.2 Proof of Theorem 2

Let us re-express CMI criterion, presented in main text’s eq. (10), using the identity \(I(A; B|C) = I(A; B|C) - I(A; C|B) - I(A; C)\):
\[J_{\text{CMI}}(X_k) = I(X_k; Y) - I(X_k; X_B) + I(X_k; X_B|Y).\] (29)

Now we will decompose the second and third term, which capture redundancy and complementarity, using Assumptions 1 and 2 respectively.

**Redundancy term** - This term can be written as:
\[I(X_k; X_B) = H(X_B) - H(X_B|X_k)\]
A.3 Proof of Theorem 3

Using Assumption 1 we can re-write the rhs as:

$$I(X_k; X_\theta) = H(X_\theta) - \sum_{X_j \in X_\theta} H(X_j|X_k) - \sum_{X_{\bar{j}} \in X_\theta} \sum_{X_j \in X_\theta} H(X_{\bar{j}}|X_k, X_j)$$

Using the identity $H(A|B) = H(A) - I(B; A)$ for the second term, and $H(A|BC) = H(A|C) - I(B; A|C)$ for the third term, the above equation can be written as:

$$I(X_k; X_\theta) = H(X_\theta) - \sum_{X_j \in X_\theta} H(X_j|X_k) + \sum_{X_{\bar{j}} \in X_\theta} \sum_{X_j \in X_\theta} I(X_{\bar{j}}; X_k|X_j)$$

**Complementarity term** - This term can be written as:

$$I(X_k; X_\theta|Y) = H(X_\theta|Y) - H(X_\theta|X_k, Y)$$

Using Assumption 2 we can re-write the rhs as:

$$I(X_k; X_\theta|Y) = H(X_\theta|Y) - \sum_{X_j \in X_\theta} H(X_j|X_k, Y) - \sum_{X_{\bar{j}} \in X_\theta} \sum_{X_j \in X_\theta} H(X_{\bar{j}}|X_k, X_j, Y)$$

Using the identity $H(A|BC) = H(A|C) - I(B; A|C)$ for the second term, and $H(A|BCD) = H(A|CD) - I(B; A|CD)$ for the third term, the above equation can be written as:

$$I(X_k; X_\theta|Y) = H(X_\theta|Y) - \sum_{X_j \in X_\theta} H(X_j|Y) + \sum_{X_{\bar{j}} \in X_\theta} \sum_{X_j \in X_\theta} I(X_{\bar{j}}; X_k|X_j|Y)$$

The derived redundancy and complementarity terms, eqs. (30) and (31), can be substituted to eq. (29) so the CMI criterion can be written as follows:

$$J_{\text{CMI}}^{\theta_k} = I(Y_k; X_k) - \sum_{X_j \in X_\theta} I(X_j; X_k) + \sum_{X_{\bar{j}} \in X_\theta} \sum_{X_j \in X_\theta} I(X_{\bar{j}}; X_k|X_j)$$

where Const are constant terms with respect to $X_k$, as such removing them will have no effect on the choice of feature. Removing these terms we have an equivalent criterion.

A.3 Proof of Theorem 3

The JMI-3 criterion can be written in the following way:

$$J_{\text{JMI-3}}(X_k) = \sum_{X_j \in X_\theta} \sum_{X_{\bar{j}} \in X_\theta} I(X_k; X_i, X_{\bar{j}}; Y) = \sum_{X_j \in X_\theta} \sum_{X_{\bar{j}} \in X_\theta} (I(X_i; X_j; Y) + I(X_k; Y|X_i, X_j))$$

The first term is constant with respect to $X_k$, as such removing it will have no effect on the choice of feature. We will use the identity $I(A; B|C) = I(A; B) - I(A; C) + I(A; C|B)$ to re-express the conditional mutual information term.
\[ J_{\text{JMI-3}}(X_k) \propto \sum_{X_j \in \mathcal{X}_0} \sum_{X_i \in \mathcal{X}_0, i \neq j} (I(X_k; Y) - I(X_k; X_i | X_j) + I(X_k; X_i X_j | Y)) \]

The last two terms of the rhs can written as follows: \( I(X_k; X_i | X_j) = I(X_k; X_i) + I(X_k; X_i | X_j) \) and \( I(X_k; X_i X_j | Y) = I(X_k; X_i | Y) + I(X_k; X_i | X_j Y) \). Thus the JMI-3 criterion is

\[ J_{\text{JMI-3}}(X_k) \propto \sum_{X_j \in \mathcal{X}_0} \sum_{X_i \in \mathcal{X}_0, i \neq j} \left( I(X_k; Y) - I(X_k; X_i | X_j) + I(X_k; X_i X_j | Y) \right) \]

\[ = \|X_0\|(|X_0| - 1) I(X_k; Y) - (|X_0| - 1) \sum_{X_j \in \mathcal{X}_0} I(X_k; X_j) - \sum_{X_j \in \mathcal{X}_0} \sum_{X_i \in \mathcal{X}_0, i \neq j} I(X_k; X_i | X_j) \]

\[ + (|X_0| - 1) \sum_{X_j \in \mathcal{X}_0} I(X_k; X_j) + \sum_{X_j \in \mathcal{X}_0} \sum_{X_i \in \mathcal{X}_0, i \neq j} I(X_k; X_i | X_j Y) \]

\[ \propto I(X_k; Y) - \frac{1}{|X_0|} \sum_{X_j \in \mathcal{X}_0} I(X_k; X_j) + \frac{1}{|X_0|} \sum_{X_j \in \mathcal{X}_0} \sum_{X_i \in \mathcal{X}_0, i \neq j} I(X_k; X_i | X_j Y) \]

The last expression shows that the JMI-3 criterion can be decomposed in the five terms of main text’s eq. (17) with coefficients: \( \beta = \gamma = 1/|X_0| \), and \( \beta' = \gamma' = 1/|X_0|(|X_0| - 1) \).

\[ \text{A.4 Proof of Theorem 4} \]

Using identity \( I(A; B|C) = I(A; B) - I(A; C) + I(A; C|B) \), we can re-express the CMIM-3 criterion in the following way:

\[ J_{\text{CMIM-3}}(X_k) = \min_{X_j \in \mathcal{X}_0} \left[ I(X_k; Y) - I(X_k; X_i | X_j) + I(X_k; X_i X_j | Y) \right] \]

\[ = I(X_k; Y) - \max_{X_j \in \mathcal{X}_0} \left[ I(X_k; X_i | X_j) - I(X_k; X_i X_j | Y) \right] \]

The last two terms of the rhs can written as follows: \( I(X_k; X_i | X_j) = I(X_k; X_i) + I(X_k; X_i | X_j) \) and \( I(X_k; X_i X_j | Y) = I(X_k; X_i | Y) + I(X_k; X_i | X_j Y) \). Thus the CMIM-3 criterion can be decomposed as follows:

\[ J_{\text{CMIM-3}}(X_k) = I(X_k; Y) - \max_{X_j \in \mathcal{X}_0} \left[ I(X_k; X_j) - I(X_k; X_i | X_j) + I(X_k; X_i X_j | Y) \right] \]

\[ \text{B Protocol for generating synthetic data} \]

\[ \text{B.1 Generating data for Section 3.2} \]

The data are generated as follows:
1. We specify the desired values for the population MI i.e. \( I(X; Y) \in (0, 0.05) \)
2. We generate the population values for the probabilities \( p(xy) \) by sampling from a Dirichlet distribution. Using these probabilities we can calculate the population value of the mutual information \( I(X; Y) \), and if it is inside the desirable values (specified in Step 1) we keep the probabilities, else we sample again. Every time we sample from a Dirichlet, \( \text{Dir}(\alpha) \), the concentration parameter \( \alpha \) is a number chosen randomly from: \([0.3 - 3]\). It is interesting to mention here that the concentration parameter \( \alpha \) controls the concentration of the prior: large \( \alpha \) provides uniform distributions, and as a result small MI values, while small values lead to more concentrated distributions, which generate higher mutual information values. Using the probabilities \( p(xy) \), we calculate \( p(x) = \sum_{y \in Y} p(xy) \), and \( p(y|x) = \frac{p(xy)}{p(x)} \).
3. We generate the values of \( X, \{x^n\}_{n=1}^N \), by sampling \( N \) data from the marginal distribution \( p(x) \). Then we generate the values of \( Y \) by sampling \( N \) data from the conditional distributions \( \{p(y|x^n)\}_{n=1}^N \).

B.2 Generating data for Section 3.3

The data are generated as follows:
1. We specify the desired values for the population CMI i.e. \( I(X; Y|Z) \in (0, 0.05) \)
2. We generate the population values for the probabilities \( p(x) \) and \( p(y) \) by sampling from a Dirichlet distribution, and for each value of \( X \) and \( Y \) we generate the values of \( p(z|xy) \) by sampling again from a Dirichlet. Using these probabilities we can calculate the population value of the conditional mutual information \( I(X; Y|Z) \), and if it is inside the desirable values (specified in Step 1) we keep the probabilities, else we sample again. Every time we sample from a Dirichlet, \( \text{Dir}(\alpha) \) the concentration parameter \( \alpha \) is a number chosen randomly from: \([0.3 - 3]\).
3. We generate the values of \( X \) and \( Y, \{x^n, y^n\}_{n=1}^N \), by sampling \( N \) data from the marginal distribution \( p(x) \) and \( p(y) \) respectively. Then we generate the values of \( Z \) by sampling \( n \) data from the conditional distributions \( \{p(z|x^n, y^n)\}_{n=1}^N \).

C Datasets Used

Table 1 shows the characteristics of the 11 benchmark BN\(^1\) that we used to simulate the data in Section 5, while Table 2 shows the details of the 20 UCI datasets\(^2\) used in Section 6.

| # | Network | Total number of nodes | Number of target nodes | Average MB size of target nodes |
|---|---------|-----------------------|------------------------|---------------------------------|
| 1. | asia    | 8                     | 4                      | 3.50                            |
| 2. | child   | 20                    | 8                      | 5                               |
| 3. | insurance | 27                    | 19                     | 6.05                            |
| 4. | water   | 32                    | 16                     | 10.25                           |
| 5. | alarm   | 37                    | 12                     | 5.42                            |
| 6. | barley2 | 48                    | 29                     | 6.48                            |
| 7. | hallfinder | 56                    | 24                     | 5.04                            |
| 8. | hep2    | 70                    | 16                     | 11                              |
| 9. | wind9pts | 76                    | 25                     | 7.76                            |
| 10. | pathfinder | 109                   | 30                     | 5.87                            |
| 11. | andes   | 223                   | 112                    | 7.32                            |

\(^1\) Downloaded from http://www.bnlearn.com/bnrepository/
\(^2\) downloaded from https://archive.ics.uci.edu/ml/datasets.html
Table 2 Summary of UCI datasets.

| #  | Name     | Examples | Features | Classes |
|----|----------|----------|----------|---------|
| 1. | lungcancer | 32       | 56       | 3       |
| 2. | soybean   | 47       | 35       | 4       |
| 3. | wine      | 178      | 13       | 3       |
| 4. | parkinsons| 195      | 22       | 2       |
| 5. | sonar     | 208      | 60       | 2       |
| 6. | spect     | 267      | 22       | 2       |
| 7. | heart     | 270      | 13       | 2       |
| 8. | liver     | 345      | 6        | 2       |
| 9. | ionosphere| 351      | 33       | 2       |
| 10.| congress  | 435      | 16       | 2       |

D Experimental Results

Tables 3 and 4 contain the complete results of Section 5 for each dataset. Table 5 contain the results presented in Section 6.

Table 3 Comparison between our suggested high-order FS criteria in terms of their ability to identify the correct features (TPR) for BN with: (a) Sample size = 500, and (b) Sample size = 2500. The best method (i.e. highest TPR) is highlighted with bold font and at the bottom of the table we present the average ranking score of each method across all datasets.

|    | JInd-JS | JMI-3 | JMI-4 | JInd-JS | JMI-3 | JMI-4 |
|----|---------|-------|-------|---------|-------|-------|
| asia| 0.798   | 0.798 | 0.808 | 0.758   | 0.828 | 0.827 |
| child| 0.773   | 0.741 | 0.661 | 0.647   | 0.804 | 0.813 |
| hailfinder| 0.497 | 0.486 | 0.450 | 0.446 | 0.556 | 0.558 |
| alarm| 0.709   | 0.733 | 0.618 | 0.671   | 0.704 | 0.777 |
| pathfinder| 0.450 | 0.428 | 0.412 | 0.373 | 0.526 | 0.497 |
| insurance| 0.634 | 0.611 | 0.618 | 0.633 | 0.683 | 0.683 |
| barley2| 0.479   | 0.444 | 0.460 | 0.408   | 0.530 | 0.510 |
| andes| 0.591   | 0.576 | 0.527 | 0.527   | 0.651 | 0.659 |
| win95pts| 0.600  | 0.578 | 0.477 | 0.445 | 0.662 | 0.684 |
| water| 0.507   | 0.492 | 0.433 | 0.388   | 0.579 | 0.570 |
| hepar2| 0.501   | 0.489 | 0.494 | 0.463   | 0.658 | 0.650 |

Avg ranking 1.227 2.318 2.727 3.727

CD diagram Figure 5(a)

|    | JInd-JS | JMI-3 | JMI-4 | JInd-JS | JMI-3 | JMI-4 |
|----|---------|-------|-------|---------|-------|-------|
| asia| 0.828   | 0.823 | 0.827 | 0.835   | 0.828 | 0.827 |
| child| 0.813   | 0.739 | 0.736 | 0.835   | 0.813 | 0.739 |
| hailfinder| 0.486 | 0.486 | 0.486 | 0.486 | 0.486 | 0.486 |
| alarm| 0.777   | 0.633 | 0.734 | 0.835   | 0.777 | 0.633 |
| pathfinder| 0.497 | 0.455 | 0.418 | 0.835   | 0.497 | 0.455 |
| insurance| 0.683 | 0.654 | 0.717 | 0.835   | 0.683 | 0.654 |
| barley2| 0.555   | 0.555 | 0.439 | 0.835   | 0.555 | 0.439 |
| andes| 0.659   | 0.600 | 0.619 | 0.835   | 0.659 | 0.600 |
| win95pts| 0.684  | 0.596 | 0.563 | 0.835   | 0.684 | 0.596 |
| water| 0.570   | 0.498 | 0.445 | 0.835   | 0.570 | 0.498 |
| hepar2| 0.650   | 0.644 | 0.618 | 0.835   | 0.650 | 0.644 |

Avg ranking 1.864 1.864 3.182 3.091

CD diagram Figure 5(b)

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Olivier Ledoit and Michael Wolf. Improved estimation of the covariance matrix of stock returns with an application to portfolio selection. Journal of empirical finance, 10(5):605–621, 2003.

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Juliane Schäfer and Korbinian Strimmer. A shrinkage approach to large-scale covariance matrix estimation and implications for functional genomics. Statistical applications in genetics and molecular biology, 4(1), 2005.
Table 4 Comparing the different feature selection methods in terms of their ability to identify the correct features (TPR) for BN with: (a) Sample size = 500 , and (b) Sample size = 2500. The best method (i.e. highest TPR) is highlighted with bold font and at the bottom of the table we present the average ranking score of each method across all datasets.

| Method | Asia | Child | Hailfinder | Alarm | Pathfinder | Insurance | Barley2 | Andes | Win95pts | Water | Hepar2 | Avg ranking | CD diagram |
|--------|------|-------|------------|-------|------------|-----------|---------|-------|----------|-------|-------|-------------|------------|
| (a) TPR with 500 sample size | | | | | | | | | | | | | |
| MIM | 0.613 | 0.638 | 0.531 | 0.480 | 0.460 | 0.560 | 0.452 | 0.477 | 0.490 | 0.481 | 0.478 | 6.364 | Figure 6(a) |
| MIFS | 0.683 | 0.746 | 0.621 | 0.480 | 0.262 | 0.488 | 0.431 | 0.422 | 0.361 | 0.382 | 0.439 | 9.955 | |
| DISR | 0.748 | 0.685 | 0.481 | 0.345 | 0.392 | 0.596 | 0.412 | 0.483 | 0.510 | 0.459 | 0.452 | 5.545 | |
| ICAP | 0.763 | 0.648 | 0.609 | 0.639 | 0.480 | 0.483 | 0.456 | 0.536 | 0.439 | 0.389 | 0.465 | 7.273 | |
| CIFE | 0.775 | 0.589 | 0.631 | 0.631 | 0.481 | 0.503 | 0.456 | 0.536 | 0.395 | 0.389 | 0.445 | 7.364 | |
| mRMR | 0.683 | 0.675 | 0.632 | 0.632 | 0.631 | 0.483 | 0.422 | 0.536 | 0.454 | 0.389 | 0.434 | 5.364 | |
| JMI | 0.755 | 0.656 | 0.621 | 0.621 | 0.632 | 0.503 | 0.474 | 0.536 | 0.473 | 0.389 | 0.515 | 1.818 | |
| CMIM relax-mRMR | 0.808 | 0.610 | 0.629 | 0.629 | 0.629 | 0.503 | 0.474 | 0.503 | 0.515 | 0.478 | 0.515 | 4.909 | |
| JMI-3 | 0.802 | 0.773 | 0.709 | 0.709 | 0.700 | 0.556 | 0.496 | 0.503 | 0.548 | 0.448 | 0.547 | 1.636 | |
| Avg ranking | | | | | | | | | | | | | |
| (b) TPR with 2500 sample size | | | | | | | | | | | | | |
| MIM | 0.625 | 0.673 | 0.503 | 0.530 | 0.485 | 0.573 | 0.452 | 0.477 | 0.510 | 0.530 | 0.592 | 7.364 | Figure 6(b) |
| MIFS | 0.700 | 0.567 | 0.439 | 0.480 | 0.290 | 0.500 | 0.428 | 0.349 | 0.409 | 0.428 | 0.447 | 10.545 | |
| DISR | 0.602 | 0.762 | 0.536 | 0.616 | 0.499 | 0.601 | 0.428 | 0.494 | 0.510 | 0.428 | 0.510 | 5.545 | |
| ICAP | 0.802 | 0.772 | 0.454 | 0.515 | 0.499 | 0.603 | 0.454 | 0.494 | 0.538 | 0.494 | 0.538 | 5.455 | |
| CIFE | 0.800 | 0.705 | 0.454 | 0.646 | 0.479 | 0.603 | 0.454 | 0.494 | 0.605 | 0.494 | 0.605 | 5.355 | |
| mRMR | 0.700 | 0.733 | 0.670 | 0.670 | 0.753 | 0.603 | 0.454 | 0.494 | 0.605 | 0.494 | 0.605 | 3.455 | |
| JMI | 0.827 | 0.614 | 0.739 | 0.739 | 0.614 | 0.603 | 0.454 | 0.494 | 0.605 | 0.494 | 0.605 | 5.364 | |
| CMIM relax-mRMR | 0.700 | 0.524 | 0.556 | 0.556 | 0.524 | 0.614 | 0.454 | 0.494 | 0.605 | 0.494 | 0.605 | 5.000 | |
| JMI-3 | 0.828 | 0.556 | 0.504 | 0.504 | 0.550 | 0.614 | 0.454 | 0.494 | 0.605 | 0.494 | 0.605 | 5.364 | |
| Avg ranking | | | | | | | | | | | | | |
| CD diagram | | | | | | | | | | | | | |
Table 5 Comparing the different FS methods in terms of their misclassification error. In brackets is the ranking score of each method in each dataset, and in the bottom of the table average ranking score of each method across all datasets.

| Method      | lungcancer | soybean-small | sonar | parkinsons | ionosphere | spect | wine | breast | heart | congress | muskel | splice | liver | spambase | krrskep | pima | waveform | landsat | mushroom |
|-------------|------------|---------------|-------|------------|------------|-------|------|--------|-------|----------|--------|--------|-------|----------|--------|------|----------|---------|---------|
| MIM         | 0.589(9)   | 0.614(14)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| MIFS        | 0.584(6)   | 0.608(8)      | 0.637(5) | 0.612(6)   | 0.605(12)  | 0.597(4) | 0.608(7) | 0.597(3) | 0.612(5) | 0.605(10) | 0.608(2) | 0.608(1) | 0.608(13) | 0.608(1) |
| DISR        | 0.589(8)   | 0.614(11)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| ICAP        | 0.584(5)   | 0.605(8)      | 0.589(10) | 0.584(6)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| CIFE        | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| CMI         | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| mRMR        | 0.605(13)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| JMI         | 0.589(11)  | 0.614(14)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| CMIM        | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| relax-MRMR  | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| JMI-3       | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| CMIM-3      | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| JMI-4       | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |
| CMIM-4      | 0.589(10)  | 0.614(13)     | 0.589(10) | 0.584(5)   | 0.605(13)  | 0.570(2) | 0.586(7) | 0.584(4) | 0.586(6) | 0.591(11) | 0.587(8) | 0.57(3) | 0.601(12) | 0.558(1) |

Avg ranking 9.30 11.05 7.85 8.70 10.40 8.40 7.15 6.05 5.50 5.90 5.80 5.10 6.70 6.10 10.00

CD diagram Figure 7