Feature Selection with Mutual Information

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Outline

Feature Selection

Why do we perform feature selection?

- Quality of the input data is just as important as the algorithm you choose
- The volume of a feature space grows exponentially in the number of dimensions $V \propto \alpha^N$
- But we often have a small number of samples

Using Mutual Information for Feature Selection

Mutual information comes from information theory and statistics.

$$
\begin{aligned}
I(X;Y) &= D_{KL}(P(X,Y)||P(X)P(Y)) \\
&= H(X) - H(X|Y)
\end{aligned}
$$

where H denotes the entropy

- It quantifies the amount of information one variable carries about another
- Is a "generalized correlation" - it is not limited to continuous random variables
- $X = \{x_i\}_{i=1}^{N}$ and Y could be categorical e.g., cellular phenotypes

Using Mutual Information for Feature Selection

For phenotyping, we might want to find the optimal X which is most informative about the cell type Y

This is just an optimization problem on maximizing the joint mutual information

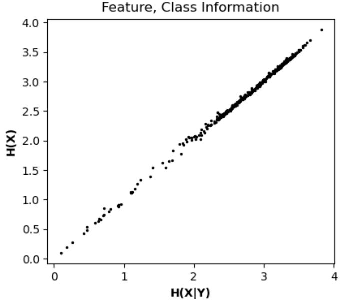
$$X^* = \underset{X}{\operatorname{argmax}} \; I(\boldsymbol{X}; Y)$$

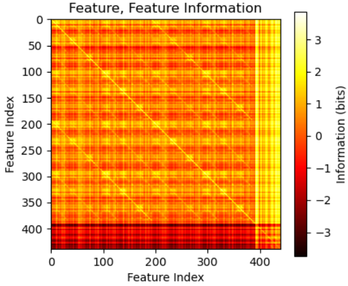
But this is a NP-hard optimization problem, but there are approximate solutions

Results for T1D dataset

Maximize:

$$I(\boldsymbol{X};Y) \approx \sum_i \left(I(X_i;Y) - \alpha \sum_j I(X_i;X_j) \right)$$





Algorithm Details

The chain-rule for mutual information tells us that

$$I(\boldsymbol{X}; Y) = \sum_i I(X_i; Y|\boldsymbol{X}_{\setminus i}) \tag{1}$$

To simplify notation let $Z = \boldsymbol{X}_{\setminus i}$. The chain rule for info can also be used to show that

$$I(X; Y, Z) = I(X; Z) + I(X; Y|Z)$$

Solving for $I(X; Y|Z)$ says we can rewrite (1) as

$$\begin{aligned} I(\boldsymbol{X}; Y) &= \sum_i I(X_i; Y|Z) \\ &= \sum_i I(X_i; Y, Z) - I(X_i; Z) \end{aligned}$$

Algorithm Details

Applying the chain rule one more time gives

$$
\begin{aligned}
I(\boldsymbol{X}; Y) &= \sum_i I(X_i; Y, Z) - I(X_i; Z) \\
&= \sum_i I(X_i; Y) - I(X_i; Z) + I(X_i; Z|Y)
\end{aligned}
$$

We maximize the sum by maximizing the each term s_i

$$
\begin{aligned}
s_i &= I(X_i; Y) - I(X_i; Z) + I(X_i; Z|Y) \\
&\approx I(X_i; Y) - \alpha \sum_j I(X_i; X_j) + \beta \sum_k I(X_i; X_k|Y)
\end{aligned}
$$

Setting $\beta = 0$ gives the so-called maximum relevancy minimum redundancy (MRMR) features

Algorithm Details

$$s_i \approx I(X_i; Y) - \alpha \sum_j I(X_i; X_j)$$

Algorithm 1 Pseudocode for Greedy MRMR

$features = \{\}$
for $i = 1$ to N **do**
    if $i = 1$ **then**
        add x_i to features
    else
        if $s_i > s_{i-1}$ **then**
            add x_i to features
        end if
    end if
end for

References I