

Simplex and S-map Algorithms

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Abstract

Pseudo-code for the simplex projection algorithm [1] and the S-map algorithm [2]. Algorithms are presented for the simple case of predicting one variable using its own time series.

1 Notation

- E denotes the embedding dimension.
- k denotes the number of nearest neighbors we use. For the simplex method, the default is $k = E + 1$ but for the S-map method it can be much larger.
- T_p denotes how many time-steps into the future we are trying to predict.
- $X \in \mathbb{R}$ denotes a (potentially long) time series.
- $y \in \mathbb{R}^E$ is a vector of lagged observations for which we want to make a prediction — in the simplest case where all components of the vector are single time step lags, y_1 represents the current value, y_2 is the value one time step prior and y_E is the value $E - 1$ time steps prior.
- $\theta \geq 0$ is the tuning parameter in the S-map method.
- $X_t^E = (X_t, X_{t-1}, \dots, X_{t-E+1})' \in \mathbb{R}^E$ denotes the lagged embedding vectors.
- $\|v\|$ is an unspecified norm of v . We do not specify which norm to use and that choice is left to the user / reader.
- $\|v\|_2^2 = \sum_i v_i^2$ is the squared L2-norm (squared Euclidean distances).
- Entries of matrices and vectors are indexed in the standard linear algebraic fashion, starting at 1 (like the R standard) and not at 0 (like the C/C++ and python standard).

2 Helper Methods

2.1 Nearest neighbors

I will not write implementation of the nearest neighbors method, just present its description. The method will be used with the signature presented in algorithm 1.

The input variables X, y and k are defined in section 1. The method returns a list of indices $N = \{N_1, \dots, N_k\}$ such that

$$\|X_{N_i}^E - y\| \leq \|X_{N_j}^E - y\| \text{ if } 1 \leq i \leq j \leq k,$$

Algorithm 1 Find Nearest neighbors

1: **procedure** NEARNEIGHBOR(y, X, k)

2.2 Least Squares

A least squares method finds x that minimizes the error in the solution of an over-determined linear system (more equations than variables). Below, $A \in \mathbb{R}^{p \times q}$, $p > q$ and $b \in \mathbb{R}^p$ and the least squares problem is to find

$$\hat{x} := \arg \min_{x \in \mathbb{R}^q} \|Ax - b\|_2^2.$$

This problem can be solved using a Singular Value Decomposition (SVD), as outlined in algorithm 2.

Algorithm 2 Least Squares via SVD

1: **procedure** LEASTSQUARES(A, b) ▷ Assume $A \in \mathbb{R}^{p \times q}$, $p > q$.
2: $U, S, V \leftarrow \text{SVD}(A)$ ▷ Thus, $A = USV'$
3: $S^{inv} \leftarrow \text{ZEROS}(q, p)$ ▷ The zero matrix in $\mathbb{R}^{q \times p}$
4: **for** $i = 1, \dots, q$ **do**
5: **if** $S_{ii} > 10^{-5} S_{11}$ **then** ▷ Note that 10^{-5} is arbitrary
6: $S_{ii}^{inv} \leftarrow \frac{1}{S_{ii}}$
7: $x \leftarrow VS^{inv}U'b$
8: **return** x

3 Simplex Projection

Ignoring ties in distances, minimal distances, minimal weights and other potential hazards, the following algorithm performs Simplex projection to predict T_p time-steps ahead.

Algorithm 3 Simplex Projection [1]

```
1: procedure SIMPLEXPREDICTION( $y, X, E, k, T_p$ )
2:    $N \leftarrow \text{NEARNEIGHBOR}(y, X, k)$   $\triangleright$  Find  $k$  nearest neighbors.
3:    $d \leftarrow \|X_{N_1}^E - y\|$   $\triangleright$  Define the distance scale.
4:   for  $i = 1, \dots, k$  do
5:      $w_i \leftarrow \exp(-\|X_{N_i}^E - y\|/d)$   $\triangleright$  Compute weights.
6:    $\hat{y} \leftarrow \sum_{i=1}^k (w_i X_{N_i+T_p}) / \sum_{i=1}^k w_i$   $\triangleright$  prediction = average of predictions.
7:   return  $\hat{y}$ 
```

4 S-map

Ignoring ties in distances, minimal distances, minimal weights and other potential hazards, the following algorithm uses the S-map method to predict T_p time-steps ahead.

Algorithm 4 S-map [2]

```
1: procedure SMAPPREDICTION( $y, X, E, k, T_p, \theta$ )
2:    $N \leftarrow \text{NEARNEIGHBOR}(y, X, k)$   $\triangleright$  Find NN to use for prediction.
3:    $d \leftarrow \frac{1}{k} \sum_{i=1}^k \|X_{N_i}^E - y\|$   $\triangleright$  Sum of distances.
4:   for  $i = 1, \dots, k$  do
5:      $w_i \leftarrow \exp(-\theta \|X_{N_i}^E - y\|/d)$   $\triangleright$  Compute weights.
6:    $W \leftarrow \text{diag}(w_i)$   $\triangleright$  Reweighting matrix.
7:    $A \leftarrow \begin{bmatrix} 1 & X_{N_1} & X_{N_1-1} & \dots & X_{N_1-E+1} \\ 1 & X_{N_2} & X_{N_2-1} & \dots & X_{N_2-E+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{N_k} & X_{N_k-1} & \dots & X_{N_k-E+1} \end{bmatrix}$   $\triangleright$  Design matrix.
8:    $A \leftarrow WA$   $\triangleright$  Weighted design matrix.
9:    $b \leftarrow \begin{bmatrix} X_{N_1+T_p} \\ X_{N_2+T_p} \\ \vdots \\ X_{N_k+T_p} \end{bmatrix}$   $\triangleright$  Response vector.
10:   $b \leftarrow Wb$   $\triangleright$  Weighted response vector.
11:   $\hat{c} \leftarrow \arg \min_c \|Ac - b\|_2^2$   $\triangleright$  Least squares, can be solved via algorithm 2.
12:   $\hat{y} \leftarrow \hat{c}_0 + \sum_{i=1}^E \hat{c}_i y_i$   $\triangleright$  Using the local linear model  $\hat{c}$  for prediction.
13:  return  $\hat{y}$ 
```

Note that k , the number of nearest neighbors used for prediction, can be very large compared to the embedding dimension E . Since $A \in \mathbb{R}^{k \times (1+E)}$, this means that A is “tall and skinny” and the system $Ac = b$ is *over-determined* (it has more equations than variables). This means (typically) that there does not exist any unique c that solves said system. This is why we seek a least-squares solution instead.

References

- [1] George Sugihara and Robert M. May. Nonlinear forecasting as a way of distinguishing chaos from measurement error in time series. *Nature*, 344:734–741, 1990.
- [2] G Sugihara. Nonlinear forecasting for the classification of natural time series. *Philosophical Transactions: Physical Sciences and Engineering*, 348(1688):477–495, 1994.