SISSO

Sure Independence Screening and Sparsifying Operator

(SISSO.3.5)

User Guide

用户指南

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Contents

1. Introduction

SISSO is a data-driven approach that combines symbolic regression and compressed sensing to identify models and descriptors in explicit mathematical expressions in materials informatics, which was originally proposed in 2018 [Phys. Rev. Mater. 2, 083802 (2018)]. Several implementations of the SISSO method are available, and this user guide is for the SISSO FORTRAN code created and maintained by Runhai Ouyang at https://github.com/rouyang2017/SISSO. Capabilities of the current SISSO code include:

➢ Regression & Classification
[R. Ouyang, S. Curtarolo, E. Ahmetcik, M. Scheffler, L. M. Ghiringhelli, Phys. Rev. Mater. 2, 083802 (2018)]

➢ Multi-task learning
[R. Ouyang, E. Ahmetcik, C. Carbogno, M. Scheffler, L. M. Ghiringhelli, J. Phys.: Mater. 2, 024002 (2019)]
[J. Wang, H. Xie, Y. Wang, R. Ouyang, J. Am. Chem. Soc. 145, 11457 (2023)]

➢ Variable selection assisted symbolic regression
[Z. Guo, S. Hu, Z.-K. Han, R. Ouyang, J. Chem. Theory Comput. 18, 4945 (2022)]

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2. Installation

A FORTRAN MPI compiler is required to compile the SISSO parallel program. Below are two options for compiling the program using an Intel MPI compiler (other compilers may work as well but the Intel compilers are recommended). Download and unzip the package in Linux operating systems, and then go to the folder 'src' and do:

1) mpiifort -fp-model precise var_global.f90 libsisso.f90 DI.f90 FC.f90 FCse.f90 SISSO.f90 -o ~/bin/SISSO

or

2) mpiifort -O2 var_global.f90 libsisso.f90 DI.f90 FC.f90 FCse.f90 SISSO.f90 -o ~/bin/SISSO

The option (1) enables better accuracy and run-to-run reproducibility of floating-point calculations; option (2) is about 2X faster than (1) but tiny run-to-run variations may happen between processors of different types, e.g. Intel and AMD.

If 'mpi' related errors present during the compilation, try opening the file 'var_global.f90' and replace the line "use mpi" with "include 'mpif.h'". However, " use mpi " is strongly encouraged (see https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report/node411.htm).

Modules of the program:

var_global.f90	! declaring the global variables.
libsisso.f90	! subroutines and functions for mathematical operations in SISSO.
DI.f90	! model sparsification (descriptor identification).
FC.f90	! feature construction with features stored in memory as numerical data.
FCse.f90	! feature construction with features stored in memory as expression tree
SISSO.f90	! the main program.

3. Running SISSO

To run SISSO for regression, classification, and multi-task learning, the two files, SISSO.in and train.dat, have to be present in the working directory. Their input templates can be found in the folder “input_templates”. The simple command-line usage is:

```
SISSO > log
```

You may need to remove resource limit by running the command 'ulimit -s unlimited'. However, users are recommended to run the code on clusters, as the SISSO jobs often require many CPU cores and much memory. For example, put this command in your submission script:

mpirun -np *number_of_cores* SISSO > log

The VS-SISSO algorithm enables symbolic regression with large number of input features, and the program VarSelect_SISSO.py (in the folder “utilities”) was created to do this job. There are calculation parameters to be defined by users in the VarSelect_SISSO.py. With the presence of the prepared SISSO.in, train.dat, and the VarSelect_SISSO.py under the working directory, users can run the VS-SISSO with the command in their submission script:

```
Python3 VarSelect_SISSO.py
```

4. Input and output files

4.1 Input files

SISSO.in

The file SISSO.in contains most of the control parameters needed to define the SISSO job on the information of the type of machine learning (regression, classification, and multi-task learning), model complexity, number of data and input features, sparsifying operators and so on. The code reads the file SISSO.in line by line to detect the keywords and corresponding values. Blank line, space, and comments starting with the exclamation mark (!) will be ignored. Users can find the template for the SISSO.in in the folder “input_templates”. Instructions on how to set the control parameters are described in the Section 5.

train.dat

There are several templates available in the folder “input_templates” for the train.dat file according to the specific machine learning job, including the train.dat_regression, train.dat_classification, train.dat_regression_multitask, and train.dat_classification_multitask. That is, users can take the train.dat template corresponding to the SISSO job defined in the SISSO.in to prepare their training data, and then rename the file as train.dat before running SISSO.

In train.dat_regression, the first line are the strings to explain/name each column. Since the second line, each line describes one data, with the first entry being a string to explain this data, e.g. compound name, the second entry being the value of the target property of this compound, and all the rest entries being the values of the input features. Each feature name is a string with maximal length of 30 characters. The special characters of space, comma, Tab, and the mathematical operators are not allowed to appear in a feature name.

In train.dat_classification, the format is the same as in the train.dat_regression, except that the second column for the target property is removed. No property values are needed for classification. SISSO only require the category information of the dataset, which will be provided in SISSO.in. For example, supposing there are the three categories A, B, C, with 50, 60, 70 data for them, respectively, you will set “nsample = (50, 60, 70)” in the SISSO.in. Correspondingly, you need to sequentially arrange the three groups of data in the train.data, i.e. the A-50 data from line 2 to 51, the B-60 data from line 52 to line 111, and the C-70 data from line 112 to line 181.

In train.dat_regression_multitask, and train.dat_classification_multitask, the formats are the same with that of train.dat_regression and train.dat_classification, respectively, except that the data are sequentially arranged task by task. For example, supposing there are the three tasks T1, T2, T3 in regression, with 100, 200, 300 data for them, respectively, then you will set “nsample = 100, 200, 300” in the SISSO.in. Correspondingly, you need to arrange the T1-100 data from line 2 to line 101, the T2-200 data from line 102 to line 301, and the T3-300 data from line 302 to line 601. In multi-task classification, supposing there are the two tasks T1 and T2, with the data (50, 60, 70) for the T1 and (80, 90, 70) for T2, then you will set “nsample = (50, 60, 70), (80, 90, 70)” in the SISSO.in, and arrange the T1-(50, 60, 70) data from line 2 to line 181, and the T2-(80, 90, 70) data from line 182 to line 421.

4.2 Output files

SISSO.out

The information of control parameters, feature spaces, and the identified best model are output to the file SISSO.out. For a SISSO-nD calculation (the model dimension is set to n in SISSO.in), the models from 1 up to n dimensions will be generated. However, the mD models ($1 \leq \mathrm{m} < \mathrm{n}$) are generated only because they are needed to generate the nD model. These mD models from the SISSO-nD calculation are often not the best as compared from calculations directly for the mD. The reason is that the computationally affordable size of the SIS-subspace for a SISSO-mD job can be far greater than that in the SISSO-nD job, and thus higher probability to get a better model. Therefore, it is recommended to perform a SISSO-xD calculation if you would like to obtain a xD model, with proper SIS-subspace size. It can be possible that when the SIS-subspace size exceeds certain threshold, the model and/or accuracy no longer change with the size, and thus convergence is reached.

To avoid confusion, only the nD model is output in SISSO.out in a nD calculation since the version v3.5.

In regression, the functional form of a nD model is $\mathrm{y} = \sum_1^n \beta_i d_i + \beta_0$, where the $\{d_i\}$ is termed the nD descriptor, $\{\beta_i\}$ are the corresponding coefficients, and β_0 is the intercept. In SISSO.out, the features_ID after each d_i is the line number of this feature in the file Uspace.expressions in the folder SIS_subspaces. In multi-task learning regression, all the tasks share the same nD descriptor, but each task have a set of different coefficients.

In classification, there are only descriptors but no coefficients in the SISSO.out. A nD descriptor means a n-dimensional map. Currently, up to 3D are implemented for classification, yet the convex-hull construction for 3D is not stable and bugs remain to be fixed. As described in Section 6.2, the classification error is defined as the amount of data in all overlap regions. The overlap size is used as the second metric in model selection. If there is no any overlap between all domains, the overlap size is given with a negative number, whose magnitude indicates the smallest separation distance between the domains. With the identified nD descriptor, one could straightforwardly apply support vector classification to find the separating hyperplanes, or decision tree to find the separating rules.

Models

This folder contains a list of the top *n* models/descriptors, where the *n* can be set in SISSO.in. The features in each model are indicated by their "Feature_ID" which is the line number in the file Uspace.expressions in the folder SIS_subspaces. For regression, coefficients are also provided in the files top*n*_D*m*_coeff, in the format of (c_i,i=0,n)_j,j=1,ntask, where c_0 is the intercept, and c_1 to c_n are the coefficients corresponding to d_1 to d_n in the linear model $\mathrm{y} = \sum_1^n c_i d_i + c_0$.

There is also the folder 'data_top1' (The 'desc_dat' in versions before v3.5) inside the 'Models'. It contains the data files of the first model in the list (It is also the model shown in the SISSO.out). The values of y_true (from the training data), y_pred (from the model prediction), and the descriptor for each training sample are provided. The file "desc_D*n*_t*m*.dat" denotes the data at dimension *n* and task *m*.

SIS_subspaces

There are *n* SIS-subspaces in a SISSO-*n*D calculation. The union of all these subspaces, including the feature expressions and feature data, are saved in the folder SIS_subspaces. The file Uspace.expressions contains the feature expressions, and the corresponding data of these expressions are provided in the file of Uspace_t*n*.dat, where the 't*n*' means the task n. For example, the features in Uspace.expressions from line 1 to N have their corresponding data in Uspace_t001.dat from column 2 to N+1 for regression (the target property occupies the first column), and from 1 to N for classification. The "t001" in the Uspace_t001.dat says that these data correspond to the task 1. The features in the Uspace.expressions are ranked according to the SIS score, i.e. the correlation between each feature and the target property.

convex$n$D_hull

In classification, each category domain is approximated by the convex volume of the data group. The file convex$n$D_hull contains the information to construct the nD volume of a data group in the space of the identified nD descriptor.

log

The log file (SISSO > log) has the progress information of a SISSO job. One can use it to monitor the progress and estimate the remaining time of the job.

VS_results

The results of performing VS-SISSO are output to the file VS_results which contains the information about the change of model errors, selected variables and other details with the iterations.

5. Control parameters

5.1 SISSO.in

The keywords in SISSO.in can be used for either regression or classification, or both. Those that are only useful for regression are noted as (R), and those only for classification are noted as (C). The (R&C) denotes the keywords are useful for both regression and classification.

ptype

ptype = 1 or 2. The type of the target property. 1: regression with continuous properties, 2: classification with categorical properties.

ntask

(R&C). **ntask** = integer. Number of tasks. **ntask** = 1: the usual machine learning with single task; **ntask** >1: multi-task learning (MTL).

task_weighting

(R). **task_weighting** = 1 (default) or 2. The weighting for MTL regression. 1: no weighting (all tasks treated equally regardless of their respective dataset size); 2: each task is weighted by $N^t/\sum_t N^t$, i.e. the amount of data in this task divided by the total amount of data in all tasks.

scmt

(R). **scmt** = .true. or .false. Sign-constrained MTL regression is invoked if .true.

desc_dim

(R&C). **desc_dim** = integer. Dimension of the descriptor/model.

nsample

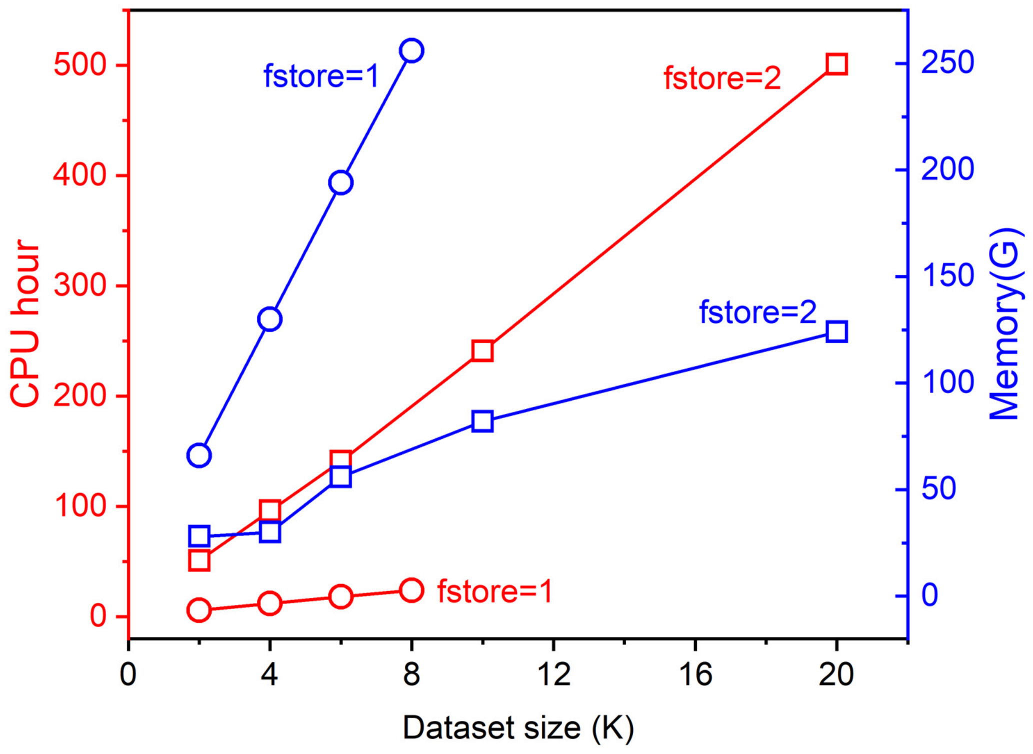
(R) **nsample** = integer, integer, …
(C) **nsample** = (integer, integer, …), (integer, integer, …), …
Number of samples in the train.dat. For single-task regression, the input is just a single integer. For MTL regression, the input is multiple integers separated by comma for the number of samples of the tasks. For single-task classification, there will be just one round bracket, inside which are the integers separated by comma for the amount of data of the corresponding categories. For MTL classification, there will be multiple round brackets separated by comma. Each bracket defines one task, and the integers inside each bracket define the amount of data for the categories.

restart

(R&C). **restart** = 0 or 1. 0: starts the job from scratch; 1: continues the job (progress information of the unfinished job is stored in the file CONTINUE)

fstore

(R&C). **fstore** = 1 or 2. 1: features are stored in memory by data (one feature, one column of data); 2: features are stored in memory by S-expression tree. Whenever needed, the feature values can be calculated on-the-fly by calling an evaluator function on the express tree. Therefore, fstore=1 is fast and high memory demand, whereas fstore=2 is low memory demand but can be several times slower than fstore=1. The figure below shows the efficiency comparison between the different scheme of feature storing in memory. If one suffer from memory problem because of too large dataset, then set fstore=2; otherwise the fstore=1 is recommended for its relatively high computational speed.



nsf

(R&C). **nsf** = integer. Number of scalar features provided in the file train.dat. The "scalar feature" means each feature is one column in the dataset.

ops

(R&C). **ops** = '(operator)(operator)(operator)…'. The mathematical operators to be used for feature construction. Users can customize the operators from the list: {+, -, *, /, exp, exp-, ^-1, ^2, ^3, sqrt, cbrt, log, |-|, scd, ^6, sin, cos}, where the "exp-", "cbrt", "|-|", "scd" means exp(-x), cubic root, |x1-x2|, and standard Cauchy distribution, respectively.

There are different rungs (maximal depth of the expression tree) during the feature construction to generate different tiers of the feature space. rung=0 (tree depth-0) corresponds to **fcomplexity** =0 (the original space of input features); rung=1 (tree depth-1) corresponds to **fcomplexity** = 1 (maximal feature complexity, i.e. number of operators in the feature, is 1; rung=2 (tree depth-2) corresponds to **fcomplexity** = 2 or 3; and rung=3 (tree depth-3) corresponds to **fcomplexity** = 4 or 5 or 6 or 7. Higher rungs require huge memory, and then the fstore=2 may be used.

The operators can be set to be the same or different in each recursion during feature construction. For example, if rung =3 (**fcomplexity** set to 4 or 5 or 6 or 7), the **ops** = '(+)(-)(*)(/)' means that the operators of +, -, *, / will be used throughout the feature construction of all recursion; and that **ops**= '(+)(-)(*)(/)', '(+)(exp)','(/)(^2)' means that the operators +, -, *, / will be used for the 1st recursion, and the + and exp will be used for the 2nd recursion, and the / and ^2 will be used for the 3rd recursion.

fcomplexity

(R&C). **fcomplexity** = integer. The feature complexity is defined as the number of operators in a feature. All the input variables and the expressions generated by mathematical combination between the input variables are all termed features. Thus, **fcomplexity**=0 means only the input variables in the feature space, and **fcomplexity**=3 means a feature space with all the features having the complexity not greater than 3. The **fcomplexity**>7 corresponds to tree depth >3 and require huge memory. In this case, **fstore**=2 can be useful to reduce the memory demand.

funit

(R&C). **funit**=(integer:integer)(integer:integer)… Each parentheses ( ) denotes one type of unit, and the integers inside the parentheses indicates that the features from n1 to n2 in the file train.dat have the same unit. For example, if in the train.dat the features from the first to the 5th have energy dimension with unit eV, features from the 6th to the 9th have the length dimension with unit angstrom, the 10th feature is dimensionless, and the 11th feature has other different unit, then in SISSO.in one can set **funit** = (1:5)(6:9)(11:11). Features not included in the **funit** are treated as dimensionless. If all input features are dimensionless, then simply comment out this line or remove the keyword **funit**. The purpose of this keyword is to enable SISSO to perform dimension analysis and avoid unreasonable combinations such as "energy + length" and "energy - length".

In SISSO, the unit of each feature is represented by a jD vector, where j is the number of unit type (number of parentheses from the input for **funit**). For example, if there are 6 features in train.dat, with their units in eV, eV, eV, Å, Å, Å, which corresponds to funit = (1:3)(4:6) in SISSO.in, then the feature units are represented by

feature1: 1 0
feature2: 1 0
feature3: 1 0
feature4: 0 1
feature5: 0 1
feature6: 0 1

The linear combinations during feature construction are only allowed between two features with the same unit vector. The unit vector (v) for the new feature generated by mathematical operations on existing features is defined as:

feature1 + feature2 and feature1 – feature2 → new_feature: v = v1 (or v2)
feature1*feature2 → new_feature: v = v1 + v2
feature1/feature2 → new_feature: v = v1 - v2

log(feature1), exp(feature1), sin(feature1), cos(feature1) $\rightarrow$ new_features: v = 0
(feature1)^n $\rightarrow$ v = v1*n

SISSO also accept the input of units from a file named “feature_units”. For example, if the units of the 6 input features are in eV, $\mathrm{eV}^{1/2}$, eV, $\mathrm{Å}^2$, $\mathrm{Å}$, $\mathrm{Å}$, then user can prepare the file in the working directory with the following content:

```
1.0    0.0
0.5    0.0
1.0    0.0
0.0    2.0
0.0    1.0
0.0    1.0
```

Please note that, when using the “feature_units” file, users have to define the **funit** parameter in SISSO.in so that the number of parenthetical arguments is equal to the number of columns in the “feature_units” file.

fmax_min

(R&C). **fmax_min** = float. The threshold that if the maximal absolute value of the data in a feature is smaller than **fmax_min**, it means the magnitudes of all numbers in the feature are so small that the feature will be treated as zero-feature and be discarded.

fmax_max

(R&C). **fmax_max** = float. The threshold that if the maximal absolute value of the data in a feature is greater than **fmax_max**, it means the magnitudes of certain numbers in the feature are so large that the feature will be treated as infinity-feature and be discarded.

nf_sis

(R&C). **nf_sis** = integer (or integer_1, integer_2, …, interger_desc_dim). Size of the SIS-subspaces. There will be n SIS-subspaces for a SISSO-nD calculation. If the input is just a single integer, then all the n subspaces have the same size. Otherwise, users can input n integers, separated by comma, to specify different size of the subspaces.

method_so

(‘L0’ for R&C, ‘L1L0’ for R only). **method_so** = ‘L0’ or ‘L1L0’. ‘L0’ is the ℓ_0-norm minimization sparsifying method. ‘L1L0’ is the method proposed by Ghiringhelli et al. [PRL 114, 105503 (2015)], i.e. firstly screening certain number of features, says 30, by using

LASSO, then followed with ℓ_0 to identify the best 1D, 2D, 3D, … models/descriptors. 'L0' is recommended for its accuracy over the 'L1L0' for low-dimensional models.

nl1l0

(R). **nl1l0** = integer. The number of features selected by LASSO for subsequent ℓ_0. Other control parameters for the LASSO are not explicitly included in the SISSO.in template. Default values for those parameters are:

L1_max_iter =1e6
The maximal number of iterations in LASSO.

L1_dens=120
Density of sampling the penalty parameter λ. The λ_i take values by using the expression: log10(λ_i) = log10(λ_{max}) – (i-1)[log10(λ_{max}) - log10(λ_{min})]/L1_dens. Here, the λ_{max} is the smallest λ for which all the coefficients are zero [J. Friedman, T. Hastie, R. Tibshirani, J. Stat. Softw. 33, (2010)], and the λ_{min} is defined as 0.001* λ_{max}.*

L1_tole =1e-6
The tolerance for the LASSO optimization with a given λ.

L1_minrmse=1e-3
The condition for LASSO to stop trial with new λ if the model LASSO_RMSE < L1_minrmse

L1_warm_start = .true.
Using the solution of last λ to start the next optimization with a new λ.

fit_intercept

(R). **fit_intercept** = .true. or .false. Fit to a nonzero / zero intercept for the linear model.

metric

(R). **metric** = 'RMSE' or 'MaxAE'. The metric for model selection in regression: RMSE (root-mean-squared error) or MaxAE (max absolute error).

nmodels

(R&C). **nmodels** = integer. Number of the top ranked models to output (see the folder 'Models').

isconvex

(C). **isconvex** = (k,k,k,…). In classification, each data domain can be restricted to be convex or nonconvex. k takes the value of 1 or 0. 1: YES; 0: NO.

bwidth

(C). **bwidth** = float. The boundary tolerance for each domain to include the data that are outside but very close to the domain.

5.2 VarSelect_SISSO.py

If one is using the VarSelect_SISSO.py to do the VS-SISSO job, then additional control parameters can be defined in the VarSelect_SISSO.py. For details about the VS-SISSO algorithm, please refer to section 6.3.

n_init = integer # Initial size for the S.

n_RS = integer # The size of the S_a.

n_max = integer # Maximal size of the S $(S = S_a + S_b)$.

nstep_max = integer # maximal iterations of the VS-SISSO

nstep_converge = integer # stop if the best model unchanged for some num. of steps.

restart = 0 or 1 # 0: start from scratch, 1: continue the job

runSISSO = '*command-to-run-SISSO***'** # E.g. 'mpirun -np 64 SISSO > log'.

6. Algorithms

6.1 Regression

As described in [Phys. Rev. Mater. 2, 083802 (2018)], the process of SISSO mainly comprises of two steps. First, feature construction. With the input variables and mathematical operators, SISSO generates all the possible 'meaningful' expressions within prescribed feature complexity (expression tree depth). Here, both the variables and expressions are all termed features, though with different feature complexity. The feature complexity is defined as the number of operators in a feature. Thus, all the input variables have complexity 0, and a feature such as $x + y/z$ has the feature complexity 2. All these features form a space, termed feature space.

Given the set of operators $\widehat{\boldsymbol{H}}$ (e.g. $\widehat{\boldsymbol{H}} = \{+, -, \times, \div, \sqrt{\square}, \exp(\square), \log(\square), ^2, \ldots\}$) and the initial feature space $\boldsymbol{\Phi}_0$ which contains all the input variables, the feature space of tier T is defined as

$$\boldsymbol{\Phi}_T \equiv \boldsymbol{\Phi}_{T-1} \bigcup \widehat{\boldsymbol{H}}[\varphi_1, \varphi_2], \qquad \forall \varphi_1, \varphi_2 \in \boldsymbol{\Phi}_{T-1}, \tag{6.1}$$

where φ_1, φ_2 are features in $\boldsymbol{\Phi}_{T-1}$ (for unary operators only φ_1 is considered). The average "+" and difference "−" operators apply to two features with the same unit. The size of $\boldsymbol{\Phi}_T$ roughly increases with $(\#\boldsymbol{\Phi}_0)^{2^T} \times (\#\widehat{\boldsymbol{H}}_2)^{2^T-1}$, where $\#\boldsymbol{\Phi}_0$ and $\#\widehat{\boldsymbol{H}}_2$ are the numbers of elements and binary operators in $\boldsymbol{\Phi}_0$ and $\widehat{\boldsymbol{H}}_2$, respectively. Thus, the size of feature space $\boldsymbol{\Phi}$ expands rapidly with the T and the number of input features in $\boldsymbol{\Phi}_0$.

Second, descriptor identification. The feature space $\boldsymbol{\Phi} = \{\varphi_i\}$ is assumed to be a basis set to expand the target property $P = \sum_i^I \beta_i \varphi_i$, and the best K features $\{\varphi_k\}$ that $P \approx \sum_k^K \beta_k \varphi_k$, $K \ll I$, are identified via sparse regression. The $\{\varphi_k\}$ is called a K-dimension descriptor. The dimension and feature complexity are the two hyperparameters defining the overall complexity of the models. Whether accurate and low-dimensional models/descriptors can exist and be identified is critically dependent on the quality of the feature space, and hence the input features, operators, as well as the reliability of the dataset.

More detailly, the algorithm is described in Figure 6.1. The model/descriptor dimension is a hyperparameter that users will test progressively from low to high until the leftover residual error is within quality expectation. For a given dimension n, SISSO will perform n iterations of the process of "feature space construction → subspace selection via sure independence screening (SIS) → descriptor identification via a sparsifying operator (SO)". In SIS, all the features of the whole feature space are firstly standardized and ranked by $|< P, \varphi_i >|$, and then the top $\#S_{1D}$ features are selected into the subspace S_{1D}. Note the standardization is only performed in SIS for the purpose of feature ranking, but not for feature construction and model building. Construction of the feature space is repeated in each iteration because the space is too large to be stored in the computer memory, and the selection of the SIS-subspace is performed on the fly. n iterations are required because n SIS-subspaces are needed to find the nD descriptor. Features in each SIS-subspace are selected based on the absolute of the inner product $|< \Delta, \varphi_i >|$, where the Δ is the residual error from previous iteration (The Δ is the P for the first iteration).

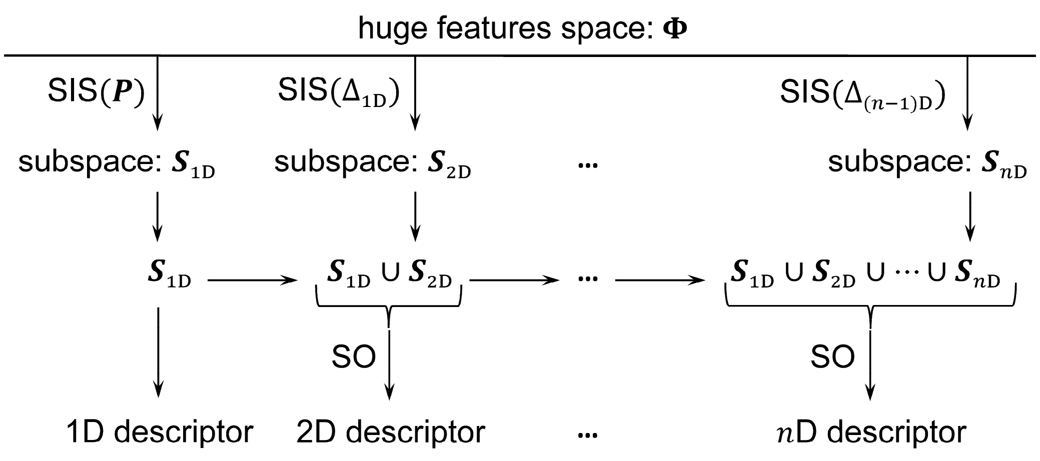

huge features space: $\boldsymbol{\Phi}$
SIS($\boldsymbol{P}$)
SIS($\Delta_{1\mathrm{D}}$)
SIS($\Delta_{(n-1)\mathrm{D}}$)
subspace: $\boldsymbol{S}_{1\mathrm{D}}$
subspace: $\boldsymbol{S}_{2\mathrm{D}}$
···
subspace: $\boldsymbol{S}_{n\mathrm{D}}$
$\boldsymbol{S}_{1\mathrm{D}}$
$\boldsymbol{S}_{1\mathrm{D}} \cup \boldsymbol{S}_{2\mathrm{D}}$
···
$\boldsymbol{S}_{1\mathrm{D}} \cup \boldsymbol{S}_{2\mathrm{D}} \cup \cdots \cup \boldsymbol{S}_{n\mathrm{D}}$
SO
SO
1D descriptor
2D descriptor
···
nD descriptor

Figure 6.1. The SISSO algorithm.

In the sparse regression, ℓ_0-norm minimization is often adopted as the SO in SISSO:

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}}(||\boldsymbol{P} - \boldsymbol{X\beta}||_2^2 + \lambda||\boldsymbol{\beta}||_0), \tag{6.2}$$

where $\boldsymbol{X}$ is union of all the SIS-subspaces selected from the $\boldsymbol{\Phi}$, and the λ is a positive tuning hyperparameter to control the model sparsity (dimension). Though the ℓ_0-norm minimization is a NP-hard problem, it remains computationally feasible if one focus on low-dimensional solutions, e.g. < 5D, with reasonable SIS-subspace size. For example, if $n = 2$, the size of each SIS-subspace can be as large as 250,000, with few hours of runtime using ~ 100 CPU cores. The total number of evaluated models by ℓ_0 is thus about C(500000,2) = $1.2*10^{11}$. Supposing $1.2*10^{11}$ is the computationally allowed largest number, if $n = 3, 4, 5$, then the corresponding size of each SIS-subspace is limited to about 3000, 330, 90, respectively. For this reason, users need to **set proper SIS-subspace size for different $\boldsymbol{n}$.** In principle, the larger the SIS-subspace, the higher probability of identifying the best models. In case $n > 10$ when each SIS-subspace can accept only 1 feature because of the limitation of computing power, SISSO becomes the orthogonal matching pursuit (OMP) method. Therefore, SISSO is a method in between the SO (SIS-subspace equal the total feature space) and the OMP (each SIS-subspace contains only 1 feature). In addition to ℓ_0, LASSO is also available as the SO for its computational efficiency, unfortunately it often yields poor results when combining with SIS.

6.2 Classification

In classification, the SISSO framework remains the same, but the definition for the loss function and the SIS are modified. In the space of descriptors, the domain of each data group/category is approximated by convex volume, as shown in Figure 6.2. Given a property with M categories, the error $||\boldsymbol{P} - \boldsymbol{X\beta}||_2^2$ in regression is replaced by the total overlap between all the M domains. The ℓ_0-norm minimization for classification is defined as:

$$\hat{\boldsymbol{c}} = \underset{\boldsymbol{c}}{\operatorname{arg}min}\left(\sum_{i=1}^{M-1}\sum_{j=i+1}^{M} O_{ij} + \lambda||\boldsymbol{c}||_0\right), \tag{6.3}$$

where O_{ij} is the number of data in the overlap region between the i and j domains, $\boldsymbol{c}$ is a sparse vector (0/1 elements) so that a feature k is selected (deselected) when c_k = 1(0), and λ is a tuning hyperparameter controlling the number of nonzero elements in $\boldsymbol{c}$.

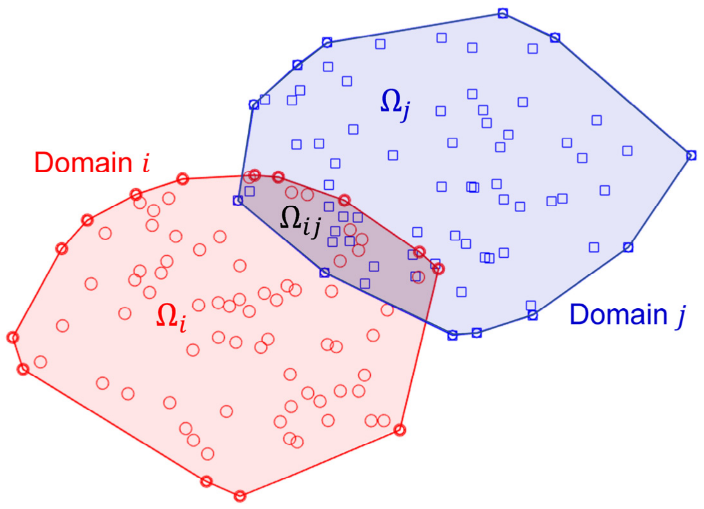


Figure 6.2. The domain for each data group is described by convex volume. The overlap area is indicated by the Ω_{ij}.

The solutions to Equation (6.3) may not be unique. Of all the possible solutions to Equation (6.3), i.e. having the same dimension and overlap-data, the one with minimal n-dimensional overlap-volume is selected:

$$\Omega \equiv \frac{2}{M(M-1)}\sum_{i=1}^{M-1}\sum_{j=i+1}^{M}\frac{\Omega_{ij}}{\min(\Omega_i,\Omega_j)}, \tag{6.4}$$

where Ω_i, Ω_j, and Ω_{ij} are the n-dimensional volumes of the i, j, and overlap ij domains. Ω has values from 0 to 1. For example, with $M = 2$, if one domain is totally included in another domain, then $\Omega = 1$; if two domains are separated, $\Omega = 0$.

In SIS for classification, the correlation between the property and a feature $|< P, \varphi_i >|$ for regression is now replaced by the $\left(\sum_{i=1}^{M-1}\sum_{j=i+1}^{M} O_{ij} + 1\right)^{-1}$ so that the higher the correlation, the lower the overlap between domains in the one-dimensional descriptor space. With the above new definitions for SIS and SO, SISSO can be applied to find the best descriptor that minimize the total overlap, or maximize the separation, between domains.

Note that above definition of error based on minimization of domain overlap is different from usual methods such as support vector classification and decision tree. Thus, the best classification model from SISSO may not work well for other methods because of their different metrics in model selection. The difference is that, SISSO not only minimize the number of misclassified data, but also minimize the misclassified domain size. With a given nD descriptor from SISSO, one can straightforwardly find the corresponding separating hyperplanes and rules by using support vector classification and decision tree, respectively.

6.3 Variable selection assisted symbolic regression

As discussed, the size of feature space $\boldsymbol{\Phi}_T$ roughly increase with $(\#\boldsymbol{\Phi}_0)^{2^T}$. Thus, increasing the number of input features will lead to rapid growth of the $\boldsymbol{\Phi}_T$. In SISSO, $\boldsymbol{\Phi}_{T-1}$ need to be stored in memory in order to generate the $\boldsymbol{\Phi}_T$. To ensure fast computation and better scaling with the number of processors, the parallelization in SISSO adopts the distributed memory system. Thus, the required memory to store the data matrix (**fstore**=1) of a feature space with M features and N samples in double precision, running on K CPU cores, is approximately $M \times N \times K \times 8/10^9$ GB. Further, each processor requires memory to store a SIS-subspace. As a result, to generate a $\boldsymbol{\Phi}_3$, with available computer memory of 256 GB and hundreds of training data, the largest size of $\boldsymbol{\Phi}_0$ is often limited to be less than 30.

To remove the limit on the size of $\boldsymbol{\Phi}_0$ and avoid huge demand of memory, a new algorithm named VS-SISSO that integrates SISSO with iterative variable selection (VS) was developed [J. Chem. Theory Comput. 18, 4945 (2022)]. The idea of VS-SISSO is shown in Figure 6.3, and the five steps are described as below.

1) Obtaining a subset Sa from the large pool of input features by random search, which has priority on unvisited features before all are visited once.
2) Let S being the union of Sa and Sb, where Sb (initially empty) is the set of variables appearing in the best model so far from symbolic regression.
3) Perform symbolic regression (SISSO) with variables in S to update the model, which has fixed complexity in all iterations.
4) Update the Sb if the training accuracy of the model is improved.
5) Stop if the accuracy converges or the iteration hits maximum; otherwise, go to step 1.

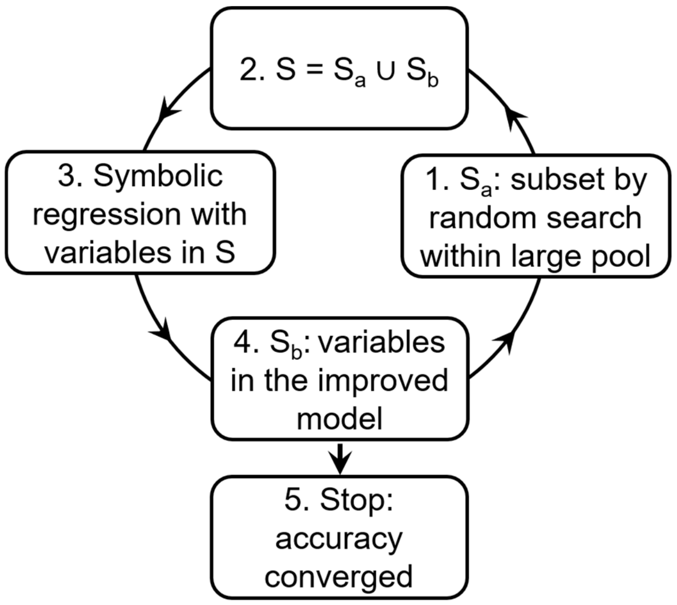

2. S = S_a ∪ S_b
3. Symbolic regression with variables in S
1. S_a: subset by random search within large pool
4. S_b: variables in the improved model
5. Stop: accuracy converged

Figure 6.3. The VS-SISSO algorithm.

6.4 Multi-task learning

Multi-task learning within the framework of SISSO (MT-SISSO) was designed to identify a common n-dimensional descriptor for several related properties [J. Phys.: Mater. 2, 024002 (2019)]. Given T properties (P^t) expanded in the same feature space $\{\varphi_i\}$, $P^t = \sum_i^N \beta_i^t \varphi_i$, the outcome of MT-SISSO learning is a common sparse model, says 2D, $P^t = \beta_1^t \varphi_1 + \beta_2^t \varphi_2$. The coefficients $\{\beta_1^t, \beta_2^t\}$ are different for different t (task), but the 2D descriptor $\{\varphi_1, \varphi_2\}$ is the same for all the tasks. With the feature space $\boldsymbol{X} = \{\varphi_i\}$ and sparsifying operator ℓ_0, the problem of regression for multi-task learning can be described as:

$$\widehat{\boldsymbol{B}} = \mathrm{arg}\underset{\boldsymbol{B}}{min} \sum_{t=1}^{T} \frac{1}{N^t} (||\boldsymbol{P}^t - \boldsymbol{X}\boldsymbol{\beta}^t||_2^2 + \lambda ||\boldsymbol{B}||_0), \tag{6.5}$$

where $\boldsymbol{X}$ are the same features for all the tasks, $\boldsymbol{B}$ is the coefficients matrix in which each column is a coefficients vector $\boldsymbol{\beta^t}$, and N^t is the number of data in the tth property $\boldsymbol{P^t}$. In Equation (6.5), all the tasks are treated equally, regardless of the dataset size for each task. The corresponding model error is defined as $\mathrm{RMSE} = \sqrt{\sum RMSE_t{}^2 / T}$, where $RMSE_t$ is the root-mean-squared error of task t. Equation (6.5) can be slightly modified so that the tasks are weighted according to their datasets size:

$$\widehat{\boldsymbol{B}} = \mathrm{arg}\underset{\boldsymbol{B}}{min} \sum_{t=1}^{T} \frac{N^t}{\sum N^t} \cdot \frac{1}{N^t} (||\boldsymbol{P}^t - \boldsymbol{X}\boldsymbol{\beta}^t||_2^2 + \lambda ||\boldsymbol{B}||_0)$$

$$= \text{arg}\underset{\boldsymbol{B}}{min}\sum_{t=1}^{T}\frac{1}{\sum N^t}(\|\boldsymbol{P}^t - \boldsymbol{X}\boldsymbol{\beta}^t\|_2^2 + \lambda||\boldsymbol{B}||_0), \tag{6.6}$$

Corresponding model error becomes $\text{RMSE} = \sqrt{\sum RMSE_t{}^2 \cdot N^t / \sum N^t}$.

In the SIS step of MT-SISSO, the correlation of each feature with the target property takes the form of quadratic mean of the $|< P^t, \varphi_i >|$ over all the tasks:

$$\theta_i = \sqrt{\sum_{t=1}^{T} < P^t, \varphi_i >^2 / T}. \tag{6.7}$$

Here, each P^t is centered (i.e. $P = P - \bar{P}$). The θ_i is further normalized by the average norm of the target property P^t: $\theta_i = \theta_i / \sqrt{\sum_t \|P^t\|^2 / N^t}$. In case of $N^t = 1$, $\theta_i = \theta_i / \|P^t\|$. Note that the P^t can not be normalized in Eq. (6.7), because they are not normalized in the equation (6.5) and (6.6). SIS ranks the features according to θ_i. Features with high θ_i are selected to form the SIS-subspaces.

Multi-task learning can also be applied to classification problems [J. Phys.: Mater. 2, 024002 (2019)]. Given T properties (tasks), the goal of multi-task learning is to find a common descriptor for T maps, in each of which the domain-overlap are minimized. The best model is obtained by minimizing the total overlap from all the maps:

$$\widehat{\boldsymbol{C}} = \text{arg}\underset{\boldsymbol{C}}{min}\left(\sum_{t=1}^{T}\sum_{i=1}^{M^t-1}\sum_{j=i+1}^{M^t} O_{ij} + \lambda||\boldsymbol{C}||_0\right). \tag{6.8}$$

The metric for SIS to evaluate the importance of a feature is defined as:

$$\theta_i = \left(\sum_{t=1}^{T}\sum_{i=1}^{M^t-1}\sum_{j=i+1}^{M^t} O_{ij} + 1\right)^{-1}. \tag{6.9}$$

6.5 Sign-constrained multi-task learning

In multi-task learning, the sign of coefficients between different tasks can be different. For example, considering the two-task 2D model $P^t = \beta_1^t\varphi_1 + \beta_2^t\varphi_2$, the first coefficient can be $\beta_1^1 < 0$ and $\beta_1^2 > 0$ for task 1 and 2, respectively. In the scenario that when MT-SISSO was applied to inconsistent multi-source experimental data, with the P^t for different tasks being the same quantity but the corresponding datasets coming from different sources (different exp. methods), it was shown that such difference of the coefficients' signs could harm the model's interpretability and predictive performance [Wang et al., J. Am. Chem. Soc. 145, 11457 (2023)]. This difficulty was solved by adding a sign-constraint to the traditional multi-task learning problem in Equation (6.5) to ensure that the coefficients between different tasks have the same signs:

$$\widehat{\boldsymbol{B}} = \underset{\boldsymbol{B}}{\operatorname{argmin}} \sum_{t=1}^{T} \frac{1}{N^t} \|\boldsymbol{P}^t - \boldsymbol{X}\boldsymbol{\beta}^t\|_2^2 + \lambda \|\boldsymbol{B}\|_0 \tag{6.10}$$

$$\text{subject to: } \operatorname{sgn}\left(\beta_j^t \cdot \beta_j^{t'}\right) \geq 0 \quad \forall\, t, t',$$

where the sgn is the sign function. This new scheme was termed sign-constrained multi-task SISSO (SCMT-SISSO). Performance of this method can be found in the work [Wang et al., J. Am. Chem. Soc. 145, 11457 (2023)].

In solving the Equation (6.10), all possible signs are tested, and the one with the lowest model error will be selected. For example, in the 2D model $P^t = \beta_1^t \varphi_1 + \beta_2^t \varphi_2$, the RMSE with ($\beta_1^t < 0,\ \beta_2^t < 0, \forall$t), ($\beta_1^t < 0,\ \beta_2^t > 0, \forall$t), ($\beta_1^t > 0,\ \beta_2^t < 0, \forall$t), and ($\beta_1^t > 0,\ \beta_2^t > 0, \forall$t) are all tested. As a result, the time cost for the sparse regression (ℓ_0) due to the sign-constraint in SCMT-SISSO will be increased by a factor of 4.

7. Utilities

Useful tools for data processing and results analysis of SISSO are provided in the folder "utilities". Explanations on how to use these tools can be found in the file Readme.