
TRAPT

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Title TRAPT: A multi-stage fused deep learning framework for transcriptional regulators prediction via integrating large-scale epigenomic data

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Description TRAPT is a multi-omics integration framework designed for inferring transcriptional regulator activity from a set of query genes. TRAPT employs a multi-stage fusion strategy to address the issues of incomplete cis-regulatory profile coverage and TRBP problems. By leveraging two-stage self-knowledge distillation to extract the activity embedding of regulatory elements, TRAPT can predicts key regulatory factors for sets of query genes through a fusion strategy.

TRAPT.CALCSAMPLERPMATRIX MODULE

TRAPT.CalcSampleRPMMatrix.**dhs2gene**(*args*, *sample*)

Calculate the Epi regulatory potential score.

Parameters

- **args** – argparse.Namespace Global parameters.
- **sample** – str Epi sample name.
- **vec** – np.array Epi PRE score.

Returns

Epi sample name, and Epi-RP score.

TRAPT.CALCTRAUC MODULE

class TRAPT.CalcTRAUC.CalcTRAUC(*args*, *RP_Matrix_TR_Sample*, *w*)

Bases: object

Calculate the area under the curve (AUC) for each TR curve.

args

Global parameters for TRAPT.

Type

TRAPT.Tools.Args

RP_Matrix_TR_Sample

The sum of TR-RP scores and D-RP scores.

Type

anndata.AnnData

w

U-RP scores.

Type

np.array

Notes

The input is the RP matrix, and the calculation is performed as follows:

$$IRP = (TRRP + DRP) \times URP$$

static get_auc(*params*)

Parallel computing module.

Parameters: *i* : int

The *i*-th row of the I-RP matrix.

j

[int] Default is 0.

labels

[np.array] Gene vector.

vec

[np.array] I-RP vector.

Returns

i, j, and the AUC score of the i-th TR.

iter_params(*gene_vec*, *trunk*)

Parallel parameter module.

Parameters: *gene_vec* : np.array

Gene vector.

trunk

[int] Number of blocks.

Returns

An iterator.

run()

TR auc calculation module execution entry point.

Returns

A pd.DataFrame of AUC scores for TRs.

TRAPT.CALCTRRPMATRIX MODULE

TRAPT.CalcTRRPMatrix.**dhs2gene**(*params*)

Calculate the TR regulatory potential score.

Parameters

- **args** – argparse.Namespace Global parameters.
- **sample** – str TR sample name.
- **vec** – np.array TR PRE score.

Returns

TR sample name, and TR-RP score.

TRAPT.CalcTRRPMatrix.**str2bool**(*v*)

TRAPT.CALCTRSAMPLERPMATRIX MODULE

```
class TRAPT.CalcTRSampleRPMMatrix.CalcTRSampleRPMMatrix(library='library', output='library',  
                                                    type='H3K27ac')
```

Bases: object

The D-RP model network aggregation module.

library

Path to the background library.

Type

str

output

Output path, default is 'library'.

Type

str

type

H3K27ac/ATAC.

Type

str

run()

D-RP model network aggregation module execution entry point.

TRAPT.DLFS MODULE

```
class TRAPT.DLFS.CustomSigmoid(*args, **kwargs)
```

Bases: Layer

```
call(x)
```

This is where the layer's logic lives.

The *call()* method may not create state (except in its first invocation, wrapping the creation of variables or other resources in *tf.init_scope()*). It is recommended to create state, including *tf.Variable* instances and nested *Layer* instances,

in *__init__()*, or in the *build()* method that is called automatically before *call()* executes for the first time.

Parameters

- **inputs** – Input tensor, or dict/list/tuple of input tensors. The first positional *inputs* argument is subject to special rules: - *inputs* must be explicitly passed. A layer cannot have zero arguments, and *inputs* cannot be provided via the default value of a keyword argument.
 - NumPy array or Python scalar values in *inputs* get cast as tensors.
 - Keras mask metadata is only collected from *inputs*.
 - Layers are built (*build(input_shape)* method) using shape info from *inputs* only.
 - *input_spec* compatibility is only checked against *inputs*.
 - Mixed precision input casting is only applied to *inputs*. If a layer has tensor arguments in **args* or ***kwargs*, their casting behavior in mixed precision should be handled manually.
 - The SavedModel input specification is generated using *inputs* only.
 - Integration with various ecosystem packages like TFMOT, TFLite, TF.js, etc is only supported for *inputs* and not for tensors in positional and keyword arguments.
- ***args** – Additional positional arguments. May contain tensors, although this is not recommended, for the reasons above.
- ****kwargs** – Additional keyword arguments. May contain tensors, although this is not recommended, for the reasons above. The following optional keyword arguments are reserved:
 - *training*: Boolean scalar tensor of Python boolean indicating whether the *call* is meant for training or inference.

- *mask*: Boolean input mask. If the layer's *call()* method takes a *mask* argument, its default value will be set to the mask generated for *inputs* by the previous layer (if *input* did come from a layer that generated a corresponding mask, i.e. if it came from a Keras layer with masking support).

Returns

A tensor or list/tuple of tensors.

class TRAPT.DLFS.**FeatureSelection**(*args*, *data_ad*, *type*)

Bases: object

TSFS(*X*, *T*)

Teacher-Student Feature Selection.

Parameters: *X* : np.array

Epi-RP matrix.

T

[str] Input genes vector.

Returns

Index values sorted by Epi sample weights, and Epi sample weights.

get_act(*t=1*)

U-RP teacher model activation function.

Parameters: *t* : float

Temperature value.

get_corr(*v1*, *v2*)

Correlation calculation.

get_loss()

U-RP teacher model loss function.

run()

U-RP model execution entry point.

Returns

A pd.DataFrame of U-RP scores for query Genes, and selected sample information.

sort_by_group(*vec*)

Grouping function.

train(*X*, *y*)

U-RP model training entry function.

Parameters: *X* : np.array

Epi-RP matrix.

y

[str] Input genes vector.

Returns

U-RP model.


```
class TRAPT.DLFS.SparseGroupLasso(l1=0.01, l2=0.01, groups=None)
```

Bases: Regularizer

```
get_config()
```

Returns the config of the regularizer.

An regularizer config is a Python dictionary (serializable) containing all configuration parameters of the regularizer. The same regularizer can be reinstantiated later (without any saved state) from this configuration.

This method is optional if you are just training and executing models, exporting to and from SavedModels, or using weight checkpoints.

This method is required for Keras *model_to_estimator*, saving and loading models to HDF5 formats, Keras model cloning, some visualization utilities, and exporting models to and from JSON.

Returns

Python dictionary.

```
TRAPT.DLFS.seed_tensorflow(seed=2023)
```


TRAPT.DLVGAE MODULE

```
class TRAPT.DLVGAE.CVAE(input_dim, condition_dim, h_dim, z_dim)
```

```
Bases: Module
```

```
forward(x)
```

```
    Defines the computation performed at every call.
```

```
    Should be overridden by all subclasses.
```

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

```
kl_div()
```

```
predict_h(x)
```

```
reparametrize(mu, logstd)
```

```
    Return type
```

```
    Tensor
```

```
training: bool
```

```
class TRAPT.DLVGAE.CalcSTM(RP_Matrix, type, checkpoint_path, device='cuda')
```

```
Bases: object
```

```
D-RP model network reconstruction module.
```

```
Parameters: RP_Matrix : TRAPT.Tools.RP_Matrix
```

```
    TR-RP matrix and Epi-RP matrix.
```

```
type
```

```
    [str] Epi-RP type.
```

```
checkpoint_path
```

```
    [str] Model save path.
```

```
device
```

```
    [str, optional] cpu/cuda.
```

```
static get_cos_similar_matrix(m1, m2)
```

```
    Matrix cosine similarity calculation.
```

get_edge_index(*A*, *B*, *n=10*)

Construct a heterogeneous network.

Parameters: *A* : `anndata.AnnData`

TR-RP matrix.

B

[`anndata.AnnData`] Epi-RP matrix.

n

[int] Number of nearest neighbors for TR.

Returns

TR-Epi heterogeneous network.

init_cvae()

D-RP teacher model training function.

init_vgae(*h*, *use_kd*)

D-RP student model training function.

Parameters: *h* : `torch.Tensor`

Potential representation of the D-RP teacher model.

use_kd

[bool] Utilize knowledge distillation.

recon_loss(*z*, *data*, *norm*, *weight*)

Variational Gaussian Autoencoder (VGAE) reconstruction loss.

run(*use_kd=True*)

D-RP model network reconstruction module execution entry point.

save_graph()

static sparse_to_tensor(*data*, *type='sparse'*)

class TRAPT.DLVGAE.InnerProductDecoderWeight(*A_e*, **args*, ***kwargs*)

Bases: `InnerProductDecoder`

forward(*z*, *edge_index=None*, *sigmoid=True*)

Decodes the latent variables *z* into edge probabilities for the given node-pairs *edge_index*.

Parameters

- *z* (`torch.Tensor`) – The latent space *Z*.
- *sigmoid* (`bool`, *optional*) – If set to `False`, does not apply the logistic sigmoid function to the output. (default: `True`)

Return type

`Tensor`

training: `bool`

class TRAPT.DLVGAE.VariationalGCNEncoder(*in_channels*, *h_dim*, *z_dim*)

Bases: `Module`

forward(*x*, *edge_index*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict_h(*x*, *edge_index*)

training: `bool`

`TRAPT.DLVGAE.seed_torch(seed=2023)`

TRAPT.RUN MODULE

`TRAPT.Run.main()`

TRAPT method entry function.

`TRAPT.Run.runTRAPT(args)`

TRAPT execution entry function.

`TRAPT.Run.args`

Global parameters for TRAPT.

Type

TRAPT.Tools.Args

`TRAPT.Run>Returns`

A `pd.DataFrame` of TR activity.

`TRAPT.Run.str2bool(v)`

TRAPT.TOOLS MODULE

```
class TRAPT.Tools.Args(input, output, library='library', threads=16, trunk_size=32768,  
                        background_genes=6000, use_kd=True, tr_type='all', source='all')
```

Bases: object

TRAPT Global Parameters.

input

Input path for the gene set.

Type
str

output

Output path for TRAPT results.

Type
str

library

Path to the background library, default is the 'library' path in the current directory.

Type
str, optional

threads

Number of processes used for TRAPT inference.

Type
int, optional

trunk_size

Size of the chunks.

Type
int, optional

background_genes

Number of background genes selected.

Type
str, optional

use_kd

Use knowledge distillation.

Type
str, optional

tr_type

all/tf/tcof/cr.

Type

str, optional

source

all/cistrome/chip_atlas/gtrd/remap/chip-atlas/remap/encode/geo.

Type

str, optional

class TRAPT.Tools.**RPMMatrix**(*library, name, to_array=True*)

Bases: object

add(*data*)

binarization()

get_data()

Return type

AnnData

minmax_scale(*axis=1*)

norm(*type='l2', axis=1*)

standard_scale(*axis=1*)

class TRAPT.Tools.**RP_Matrix**(*library*)

Bases: object

class TRAPT.Tools.**Type**

Bases: object

ATAC = 'ATAC'

H3K27ac = 'H3K27ac'

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