KLT picker 1.0 – user guide

Amitay Eldar[*], Boris Landa, Yoel Shkolnisky[†]

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1 Downloading and running the KLT picker

1.1 MATLAB package (source code)

Running the KLT picker from its source code requires MATLAB to be installed on your system.

Download and extract the package from

<div align="center">

https://github.com/amitayeldar/KLTpicker

</div>

The extracted directory has the following structure:

KLTpicker_start	Main script
userManual	Documentation for the package
LICENSE	Package license
README	A short README file
matlab/	MATLAB source code
get10028	Script to download micrographs for the example of Section 3.
example/	Directory used in Section 3 to demonstrate the KLT picker

After downloading the package, start MATLAB in the directory of the KLTpicker package and run

<div align="center">

KLTpicker_start

</div>

Using the KLT picker once started is described in Section 2.

1.2 Standalone application

The standalone package is a compiled standalone MATLAB program, and does not require MATLAB to be installed on your system. The required MATLAB runtime environment will be installed during the following installation process.

1. Download the KLT picker installer from

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[*]amitayeldar@mail.tau.ac.il

[†]yoelsh@tauex.tau.ac.il

<center>https://sites.google.com/site/yoelshkolnisky/software</center>

(only available for Linux 64 bit systems).

2. `cd` into the directory to which the installer was downloaded.

3. Make sure the installer is runnable by typing

<center>`chmod a+x ./KLTInstaller_web.install`</center>

4. Run the installer

<center>`./KLTInstaller_web.install`</center>

The installation process requires specifying two folders:

(a) Destination folder to install the KLT picker, denoted below by `<KLTfolder>`

(b) Destination folder for MATLAB Runtime, denoted below by `<MCRfolder>`

5. Once installation is done, run the KLT picker using

<center>`<KLTfolder>/application/run_KLTpicker.sh <MCRfolder>/v95`</center>

`run_KLTpicker.sh` is a shell script for temporarily setting environment variables and executing the application.

Using the KLT picker once started is described in Section 2.

2   Using the KLT picker

The following questions will appear, one by one

`Enter full path of micrographs MRC file:`

Type the path to the directory which contains the micrographs MRC files.

`Enter full path of output directory:`

Type the path where the particles coordinate files will be saved.

`Enter the particle size in pixels:`

Type the particle diameter in pixels (more precisely, the diameter of the extracted box).

`pick all particles?(Y/N)? [Y]`

Type `Y` to pick all particles using the optimal threshold derived on the paper. If you type `N`, then the following question will appear

`How many particles to pick:`

<center>2</center>

Type the number of particles to pick in each micrograph.

`Pick noise images?(Y/N)? [N]`

Type `N` if you don't want to pick noise images. If you type `Y` then the following question will appear

`How many noise images to pick:`

Type the number of noise images to pick in each micrograph.

`Do you want to use the GPU?(Y/N)? [Y]`

Type `Y` to use the GPUs found on your system, and `N` to not use them (CPU only).

The KLT picker will then start and will display progress notifications. The outputs are the coordinate files (box and star) and a text file summarizing the picking process at the output directory.

3   Example

In this section we demonstrate the use of the KLT picker on 5 micrographs of the EMPIAR-10028 data set (Plasmodium Falciparum 80S ribosome) [2] from the EMPIAR repository [1].

If MATLAB is installed, start MATLAB in the package directory and run

`get10028 # downloading 5 micrographs to ./example/micrographs directory.`

If MATLAB is not installed, download the micrographs manually from

`https://www.ebi.ac.uk/pdbe/emdb/empiar/entry/10028/`

Start the KLT picker as described in Section 1. For example, if MATLAB is installed, type

`KLTpicker_start`

Once starting the KLT picker, enter the following input

`Enter full path of micrographs MRC file:  ./example/micrographs/`

`Enter full path of output directory:  ./example/results`

`Output directory does not exist.  Create?(Y/N)? [Y] Y`

`Enter the particle size in pixels:  300`

`pick all particles?(Y/N)? [Y] Y`

```
Pick noise images?(Y/N)? [N] N
```

```
Do you want to use the GPU?(Y/N)? [Y] Y
```

Once the KLT picker has finished, it will display the massage: `Finished the picking successfully`. In order to display the picking results in EMAN [3], open a terminal in the package directory and create a new directory named `eman`, using the command

```
mkdir eman
```

Change directory to `eman` and enter the following commands one by one:

```
e2rawdata.py ../example/micrographs/*.mrc --invert --edgenorm
--xraypixel --ctfest --apix=1.0 --voltage=200.0 --cs=2.0 --ac=10.0
--threads=4 --defocusmin=0.6 --defocusmax=4.0
```

```
e2import.py
../example/results/pickedParticlesParticleSize300/box/*.box
--import_boxes --box_type=boxes
```

```
e2boxer.py --allmicrographs --boxsize=300 --ptclsize=300 --apix=1.0
--no_ctf --gui --threads=4
```

In order to display the picking results of the **first** micrograph in RELION [4], open the terminal in the package directory and create a new directory named `relion`, using the command

```
mkdir relion
```

Change directory to `relion` and enter the following command

```
relion_display --i ./example/micrographs/001.mrc --coords
./example/results/pickedParticlesParticleSize300/star/001.star
--scale 0.15 --particle_radius 150 --angpix 1 --lowpass 20 --pick
```

In order to display the picking results of the n'th micrograph change `001.mrc` and `001.star` in the above command to `00n.mrc` and `00n.star`.

4   Citation

If you use the KLT picker, please cite *KLT picker: Particle picking using data-driven optimal templates*, available at `https://arxiv.org/abs/1912.06500`.

References

[1] Iudin, A., Korir, P., Salavert-Torres, J., Kleywegt, G., and Patwardhan, A. (2016). *EMPIAR: A public archive for raw electron microscopy image data.* Nature Methods, 13.

[2] Wong, Wilson and Bai, Xiao-chen and Brown, Alan and Fernandez, Israel S and Hanssen, Eric and Condron, Melanie and Tan, Yan Hong and Baum, Jake and Scheres, Sjors H W. (2014). *Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine.* Wong et al. eLife ,3,e03080.

[3] G. Tang, L. Peng, P.R. Baldwin, D.S. Mann, W. Jiang, I. Rees & S.J. Ludtke. (2007). *EMAN2: an extensible image processing suite for electron microscopy.* Journal of structural biology, 157, 38-46.

[4] Scheres, Sjors HW. (2015). *Semi-automated selection of cryo-EM particles in RELION 1.3.* Journal of structural biology, 128, 114-122.