Star Dust XRF File Conversion

Version: version 1

Prepared for: American Museum of Natural History

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Problem Description

Objective

To convert existing x-ray data files into a readable formats, specifically netcdf (h5), that can be imported into into GSECARS Mapviewr, one of the tools in the Larch application suite.

Technical Requirements

File Format 1

xmap: XRF spectra saved to NetCDF by the Epics MCA detector
struck: a multichannel scaler, saved as ASCII column data
xps: stage positions, saved as ASCII file from the Newport XPS

Scan.ini - scan configuration file
ROI.dat - ROI definitions
Environ.dat - Extra Epics PV name/values at start of scan
Master.dat - values of "slow positioner" and scan files per row

xps.NNNN - Position of stages from XPS for row NNNN
struck.NNNN Ion Chamber intensities for row NNNN xmap.NNNN XRF spectra for row NNNN (netcdf)

File Format 2:
XRF

Approach

(1) Identify the format of the files provided by AMNH
(2) Find and Assess potential tools and existing packages
(3) Develop code to ingest the data from the above file formats
(4) Develop code that outputs the data the ingested data, i.e. associated spectra value
    a. as a netcdf file
    b. can be impoerted uusing
(5)

Proposed Solution

References:

American Museum of Natural History Hackathon: Track The Stardust Challenge:
https://github.com/amnh/HackTheSolarSystem/wiki/Track-The-Stardust

XAS Data Interchange Format Draft Specification

Github: https://github.com/XraySpectroscopy/XAS-Data-Interchange

Command:

```
        file -m magic <enter filename/path here>
```

```
FullXRF_T152_FullMap1_001/1001_001.xrf:   ASCII text, with CRLF line
terminators

T102_alltrack_001/Environ.dat: ASCII text
T102_alltrack_001/Master.dat:  ASCII text
T102_alltrack_001/ROI.dat:     ASCII text
T102_alltrack_001/Scan.ini:    ASCII text
T102_alltrack_001/struck.0001: ASCII text
T102_alltrack_001/xmap.0001:   NetCDF Data Format data
T102_alltrack_001/xps.0001:    ASCII text
```

Larch: Data Analysis Tools for X-ray Spectroscopy

Description

Larch is an open-source toolkit for analyzing X-ray spectroscopy and scattering data as collected at modern synchrotrons X-ray sources. Larch provides general-purpose tools for visualization and analysis of numerical scientific data, and state-of-the-art tools for working with X-ray absorption and fluorescence spectroscopy data. These tools include a few graphical user interfaces for doing the most common visualization and analysis tasks and a comprehensive library of lower level functionality for more complicated analysis and for scripting.

Larch has several related target application areas:

- XAFS analysis, becoming version 2 of the Ifeffit Package for EXAFS analysis.
- Visualizing and analyzing micro-X-ray fluorescence and X-ray diffraction maps.
- Quantitative X-ray fluorescence analysis.
- Data collection software for synchrotron data.

Documentation: http://xraypy.github.io/xraylarch
Code: http://github.com/xraypy/xraylarch

Applications and Programs installed with Larch*

Application Name	GUI / CLI	Description
larch	CLI	simple command-lne interface
larch_gui	GUI	enhanced command-lne interface with data browser
gse_mapviewer	GUI	XRF Map Viewer for GSECARS X-ray microprobe data.
xas_viewer	GUI	Display XANES data, and Pre-edge Peak Fitting.
xrfdisplay	GUI	Display and analyze XRF Spectra.
Dioptas	GUI	Display XRD images, calibrate to XRD patterns.
1D XRD Viewer	GUI	Display and work with 1-D XRD patterns (beta).
2D XRD Viewer	GUI	Display XRD images (beta)
feff6l	CLI	Feff 6 EXAFS calculations
feff8l	CLI	Feff 8 EXAFS calculations - no XANES

* Note: GUI = Graphical User Interface, CLI = Command Line Interface, and *beta* indicates a work in progress.

Additional References

X-ray Fluorescence Analysis with Larch: X-ray Fluorescence Analysis with Larch

Getting Started with Larch: https://xraypy.github.io/xraylarch/getting_started.html

Comments:

- Larch is under active and open development, and has support from the U. S. National Science Foundation.
- Larch has a function that can read MCA data – the Github includes an XRF file with a similar format to the .XRF files provided: https://github.com/xraypy/xraylarch/blob/master/examples/xrf/axorf4_21kev_i050.xrf
-
- `read_gsemca()` function

  Read a GSECARS MCA spectra file, returning a Group

  Parameters: **filename** – name of GSECARS MCA file

  The returned Group has the following components:

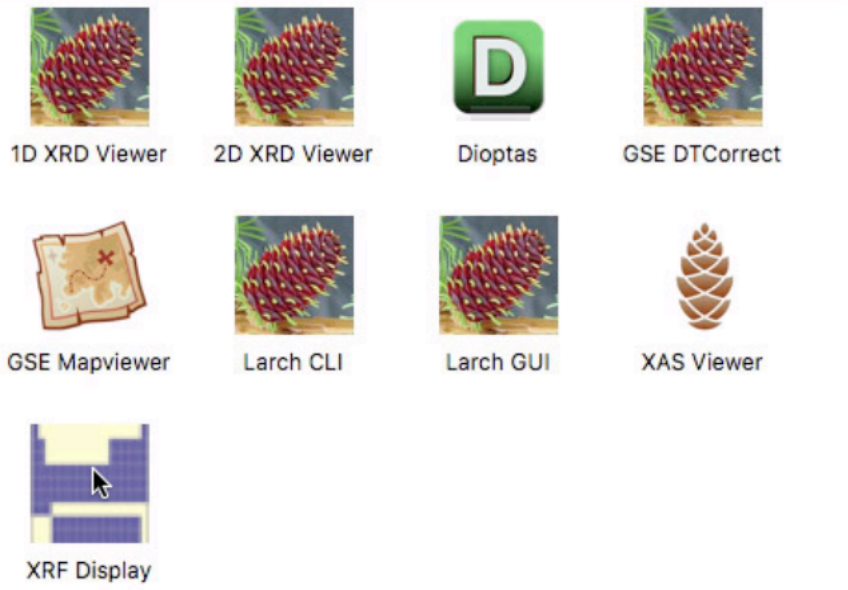
component name	description
filename	name of file
mcas	list of MCA objects for each MCA saved in the file
rois	list of ROIs
environ	list of Environmental Variables
energy	array of energy values
counts	array of counts, deadtime corrected and summed over MCAs
raw	array of counts, summed over MCAs, not corrected.
calib	dictionary of calibration values
dt_factor	deadtime correction factor
real_time	real time for data acquisition
live_time	live time for data acquisition
nchans	number of energy points in spectra
get_roi_counts()	function to get counts for a named ROI
save_mcafile()	function to save MCA to file

-

Instructions

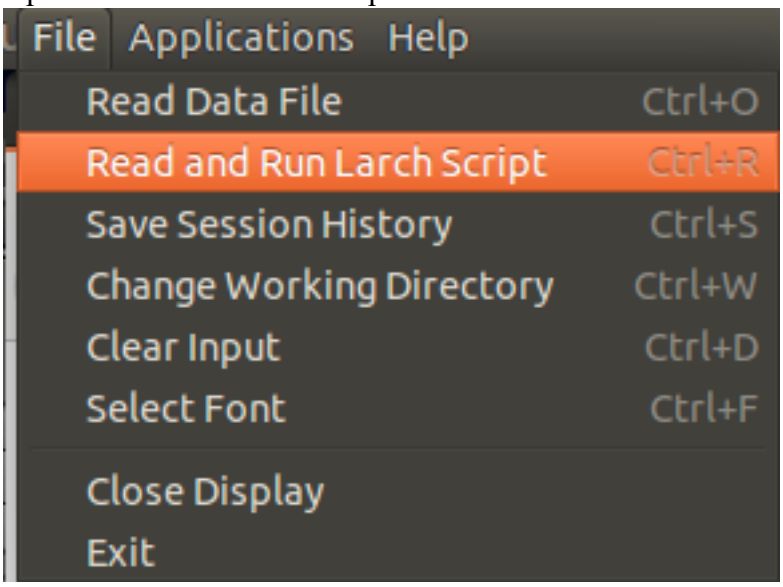
Install Larch

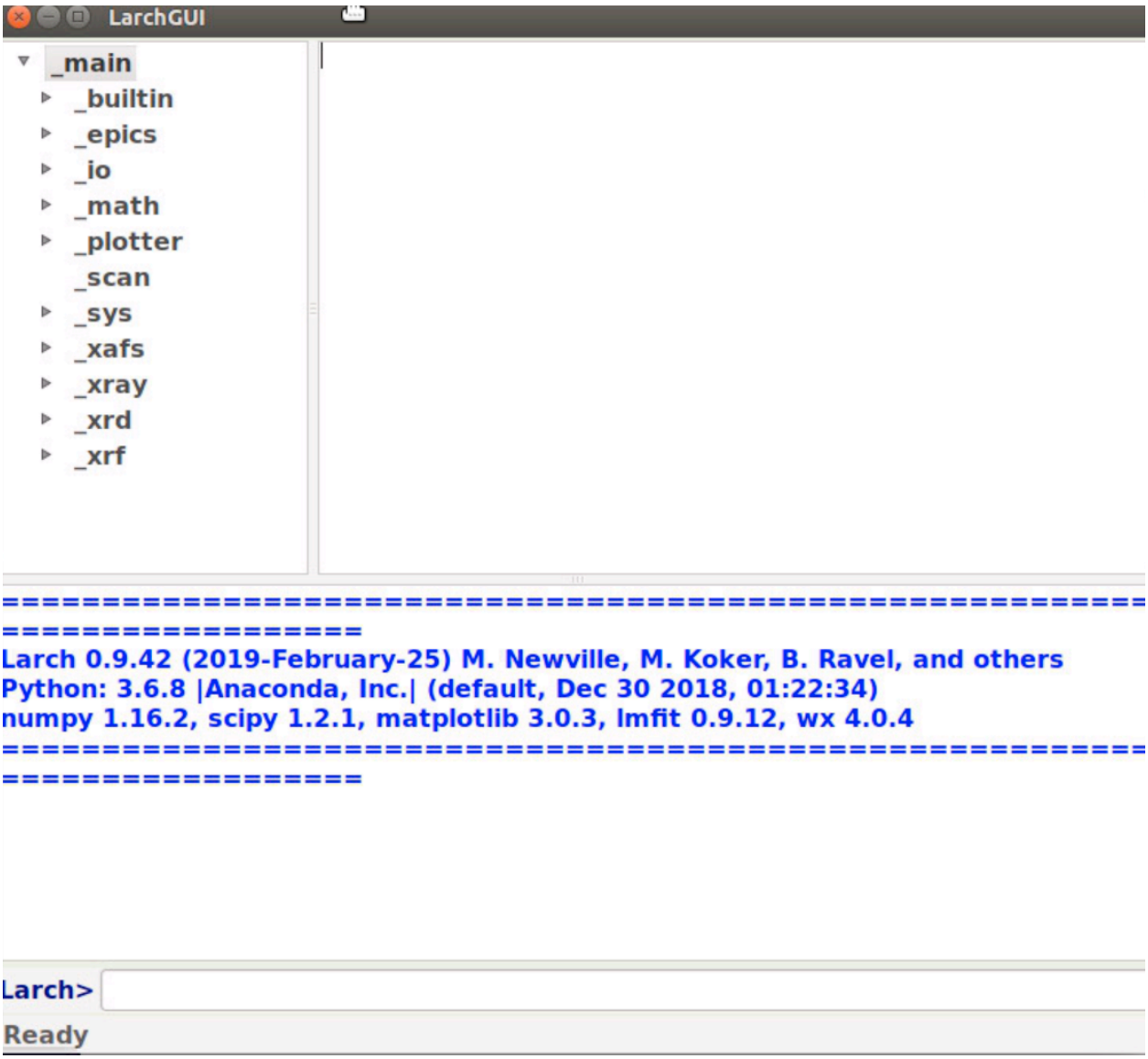
Got to the Larch folde on your desktop and open the Larch GUI



Download Larch script:
https://drive.google.com/file/d/1ir-qyTv5yhXLsy2IpiWSjWALWFnqddT5/view?usp=sharing

Open GUI and run larch script:





New functions will now appear on the GUI

At the bottom of the GUI screen, enter: Go to the GUI and enter:

get_mcalist('<name of folder with xrf files>')
get_xrflist('<name of folder with xrf files>')

The script will generate a list of the XRF files in the folder specified as the input.

Other Packages, Tools, and Resources:

FabIO

FabIO is a Python module for reading and handling data from two-dimensional X-ray detectors.

Description:
FabIO is a Python module written for easy and transparent reading of raw two-dimensional data from various X-ray detectors. The module provides a function for reading any image and returning a :class:`FabioImage` object which contains both metadata (header information) and the raw data. All FabioImage object offer additional methods to extract information about the image and to open other detector images from the same data series.

Github: https://github.com/silx-kit/fabio/blob/master/doc/source/getting_started.rst

fisx

mcareader

A minimal python interface to read Amptek's mca files.

GITHUB: https://github.com/Dih5/mcareader

PyFAI

Fast Azimuthal Integration using Python

https://pyfai.readthedocs.io/en/latest/index.html

pymca

Description
Python applications and toolkit for X-ray fluorescence analysis
PyMca is set of applications and Python libraries for analysis of X-ray fluorescence spectra.

Stand-alone application and Python tools for interactive and/or batch processing analysis of X-Ray Fluorescence Spectra. Graphical user interface (GUI) and batch processing capabilities provided.

Download [stand alone]: http://pymca.sourceforge.net

Github: https://github.com/maurov/pymca

pyepics
Python interface to Epics Channel Access

GITHUB: https://github.com/pyepics/pyepics
https://cars9.uchicago.edu/software/python/pyepics3/installation.html

pyxray

The XDI distribution contains the specification documents and various implementations of a formally specified system for reading and writing files containing single-scan XAS data.

Github: https://github.com/xrayio/pyxray

rampy

Rampy is a Python library that aims at helping processing spectroscopic data, such as Raman, Infrared or XAS spectra. It offers, for instance, functions to subtract baselines as well as to stack, resample or smooth spectra. It aims at facilitating the use of Python in processing spectroscopic data. It integrates within a workflow that uses Numpy/Scipy as well as optimisation libraries such as lmfit or emcee, for instance.

Github: https://github.com/charlesll/rampy

Description

The PyEpics module includes both low-level (C-like) and higher-level access (with Python objects) to the EPICS Channnel Access (CA) protocol. Python's ctypes library is used to wrap the basic CA functionality, with higher level objects on top of that basic interface. This approach has several advantages including no need for extension code written in C, better thread-safety, and easier installation on multiple platforms.

```
  sh build_package.sh pyepics
```

xraylib

Github: https://github.com/tschoonj/xraylib/wiki
Installation: https://github.com/tschoonj/xraylib/wiki/Installation-instructions

PyFAI

PyFAI is relying on the full Python scientific stack which includes [NumPy], [SciPy], [Matplotlib], [PyOpenCL] but also on some ESRF-developped code:

FabIO

PyFAI is using FabIO everywhere access to a 2D images is needed. The *fabio_viewer* is also a lightweight convenient viewer for diffraction images. It has been described in doi:10.1107/S0021889813000150

PyMca

The X-ray Fluorescence Toolkit provides convenient tools for HDF5 file browsing and mask drawing. It has been described in doi:10.1016/j.sab.2006.12.002

Silx

The silx toolkit is currently ongoing development. Future releases of pyFAI will use its input/output and graphical visualization capabilities

Appendix

Appendix A

File Format Examples

/T102_alltrack_001/scan.ini

```
# FastMap configuration file (saved: Sun Feb 23 02:49:53 2014)
#------------------#
[general]
mapdb = 13XRM:map:
struck = 13IDE:SIS1:
scaler = 13IDE:scaler1
xmap = 13SDD1:
mono = 13IDA:
fileplugin = netCDF1:
basedir = //Volumess/Data/xas_user/2013.2/_Setup
scandir = Scan00001
envfile = /Volumes/Data/xas_user/config/IDE_SDD1_ENV.DAT
#------------------#
[xps]
host = 164.54.160.180
user = Administrator
passwd = Administrator
group = FINE
positioners = X, Y, THETA
#------------------#
[scan]
filename = T102_alltrack.001
dimension = 2
comments =
pos1 = 13XRM:m1
start1 = -0.9
stop1 = 0.17
step1 = 0.001
time1 = 160.5
pos2 = 13XRM:m2
start2 = -0.126
stop2 = 0.066
step2 = 0.001
#------------------#
[beam_ok]
shutter_open = 13IDA:OpenFEShutter.PROC & 13IDA:OpenEShutter.PROC
shutter_status = 13IDA:eps_mbbi25   & 13IDA:eps_mbbi27
flux_val_pv = 13XRM:ION:FluxOut
flux_min_pv = 13XRM:ION:FluxLowLimit
#------------------#
[fast_positioners]
1 = 13XRM:m1 | X
2 = 13XRM:m2 | Y
3 = 13XRM:m3 | Theta
#------------------#
[slow_positioners]
1 = 13XRM:m1 | X
2 = 13XRM:m2 | Y
3 = 13XRM:m3 | Theta
4 = 13XRM:pm2 | Stage X
```

```
5 = 13XRM:m6 | Stage Y (vert)
6 = 13XRM:pm1 | Stage Z (focus)
#------------------#
```

/T102_alltrack_001/Environ.dat

/T102_alltrack_001/Master.dat

/T102_alltrack_001/ROI.dat

/T102_alltrack_001/struck.0001

/T102_alltrack_001/xmap.0001

/T102_alltrack_001/xps.0001

FullXRF_T152_FullMap1_001/001_001.xrf

```
VERSION:    3.1
ELEMENTS:   4
DATE:       Wed Jun 03 11:12:46 2009
CHANNELS:   2048
REAL_TIME:  1.000000 1.000000 1.000000 1.000000
LIVE_TIME:  1.000000 1.000000 1.000000 1.000000
CAL_OFFSET: -7.889182e-03 1.150115e-02 -2.281795e-02 -2.428983e-02
CAL_SLOPE:  1.388549e-02 1.392183e-02 1.396579e-02 1.397259e-02
CAL_QUAD:   0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
ROIS:      15 15 15 15
ROI_0_LEFT:  118 116 118 118
ROI_0_RIGHT:  132 130 132 132
ROI_0_LABEL: SiKa &  SiKa &  SiKa &  SiKa &
ROI_1_LEFT:  230 228 230 230
ROI_1_RIGHT:  247 245 247 247
ROI_1_LABEL: Kka &  Kka &  Kka &  Kka &
ROI_2_LEFT:  254 252 254 254
ROI_2_RIGHT:  275 273 274 274
ROI_2_LABEL: Ca Ka &  Ca Ka &  Ca Ka &  Ca Ka &
ROI_3_LEFT:  313 311 312 312
ROI_3_RIGHT:  335 333 334 334
ROI_3_LABEL: Ti Ka &  Ti Ka &  Ti Ka &  Ti Ka &
ROI_4_LEFT:  377 375 376 376
ROI_4_RIGHT:  402 400 401 401
ROI_4_LABEL: Cr Ka &  Cr Ka &  Cr Ka &  Cr Ka &
ROI_5_LEFT:  415 413 414 414
ROI_5_RIGHT:  436 433 435 434
ROI_5_LABEL: Mn Ka &  Mn Ka &  Mn Ka &  Mn Ka &
ROI_6_LEFT:  445 442 444 443
ROI_6_RIGHT:  480 477 478 478
ROI_6_LABEL: Fe Ka &  Fe Ka &  Fe Ka &  Fe Ka &
ROI_7_LEFT:  528 525 526 526
ROI_7_RIGHT:  550 547 548 548
ROI_7_LABEL: NiKa &  NiKa &  NiKa &  NiKa &
ROI_8_LEFT:  570 567 568 568
ROI_8_RIGHT:  592 589 590 589
ROI_8_LABEL: CuKa &  CuKa &  CuKa &  CuKa &
ROI_9_LEFT:  609 606 607 606
ROI_9_RIGHT:  637 634 634 634
ROI_9_LABEL: ZnKa &  ZnKa &  ZnKa &  ZnKa &
ROI_10_LEFT:  733 730 730 730
ROI_10_RIGHT:  783 780 780 779
ROI_10_LABEL: As Ka &  As Ka &  As Ka &  As Ka &
ROI_11_LEFT:  842 838 838 838
ROI_11_RIGHT:  870 866 866 866
ROI_11_LABEL: BrKa &  BrKa &  BrKa &  BrKa &
ROI_12_LEFT:  1000 996 995 995
ROI_12_RIGHT:  1040 1036 1035 1035
ROI_12_LABEL: Sr Ka &  Sr Ka &  Sr Ka &  Sr Ka &
ROI_13_LEFT:  1118 1114 1113 1112
ROI_13_RIGHT:  1151 1147 1145 1145
ROI_13_LABEL: ZrKa &  ZrKa &  ZrKa &  ZrKa &
ROI_14_LEFT:  1495 1490 1487 1487
ROI_14_RIGHT:  1560 1555 1552 1551
ROI_14_LABEL: elastic &  elastic &  elastic &  elastic &
DATA:
 0 0 0 0
 3 1 0 7
 5 0 1 1
 4 0 1 7
 8 1 3 5
```

5 1 2 7
2 1 1 5
6 1 2 9
10 1 0 6
3 0 2 1
3 2 1 1
5 0 0 1
2 0 0 3
0 1 1 1
0 0 0 0
0 0 0 0
1 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 0 0 0
0 1 0 0
2 2 0 1
0 1 1 3
1 1 0 1
0 1 0 0
0 0 1 0
0 3 1 1
2 1 1 2
0 1 0 0
2 0 1 1
0 2 1 0
2 0 1 0
0 1 0 0
0 0 0 2
0 0 1 0
0 0 0 1
0 1 0 0
1 1 1 0
0 0 0 1
0 1 0 1
0 0 0 0
1 1 0 0
0 0 1 0
1 2 4 1
1 0 2 0
1 0 0 1
1 0 0 0
2 5 0 1
0 1 0 1
0 2 0 1
1 1 0 2
0 1 0 0
2 2 1 0

0	0	2	0
1	0	2	0
0	3	0	0
0	0	3	3
1	2	0	0
1	1	0	0
1	0	0	1
2	1	0	0
1	0	0	0
0	0	0	0
1	0	0	1
0	2	0	1
0	2	0	0
0	1	1	0
1	1	1	0
2	1	0	0
1	1	0	1
0	2	0	1
0	0	1	0
1	0	0	3
0	1	0	0
0	1	0	0
1	1	0	3
0	0	1	0
1	1	1	1
0	1	1	0
0	0	0	0
1	0	2	1
2	0	1	0
0	0	0	1
1	0	1	0
2	0	2	0
0	0	0	1
1	0	2	0
2	0	1	0
0	2	1	0
0	1	0	0
1	0	0	0
0	0	1	0
2	1	0	0
0	0	1	0
0	0	0	0
0	0	0	1
0	2	2	0
0	1	0	0
0	0	0	1
0	1	1	0
0	1	0	0
0	0	0	0
2	1	0	1
2	1	2	0
0	1	1	1
1	2	0	0
0	1	0	0
0	1	0	0
0	1	1	0
3	0	0	1
1	0	1	0
1	0	0	0
0	0	1	0
2	1	0	0
2	1	0	1
2	0	1	1

0	2	0	2
0	0	0	0
1	0	0	0
0	0	0	0
0	0	1	1
1	0	0	0
1	1	0	0
0	3	1	1
1	1	0	0
1	0	0	1
0	0	0	1
0	0	0	1
0	1	0	0
0	0	0	1
0	1	0	0
0	0	0	0
0	1	0	1
1	0	1	0
2	0	1	0
1	0	1	0
0	0	0	0
1	0	0	0
0	0	0	0
0	0	1	1
0	0	2	0
0	1	0	0
0	0	1	1
1	0	0	0
0	0	0	0
0	1	2	0
0	0	1	0
0	0	0	1
1	0	0	0
0	0	1	0
0	1	0	0
0	1	0	0
0	1	0	0
0	0	0	0
0	0	0	0
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0	0	1	0
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1	0	0	0
0	0	0	0
1	1	0	0
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0	0	0	0
0	0	1	0
0	0	0	0
1	0	0	0
0	0	0	0
0	1	0	1
0	2	0	1
0	0	0	0
0	0	0	0
1	0	0	0
0	1	0	0
0	0	0	0
2	0	0	0
1	1	0	0
0	1	1	0
0	0	1	0

1	0	0	1
0	2	3	2
0	1	0	0
1	0	1	0
0	0	0	0
3	0	0	2
0	0	0	1
0	0	0	0
1	1	1	0
0	2	0	0
1	1	1	1
2	1	0	0
0	3	2	2
5	6	3	5
3	1	4	3
1	2	5	6
7	11	5	3
3	6	4	11
4	5	6	6
6	8	7	6
4	4	6	4
3	5	10	0
4	4	9	1
4	3	4	2
3	3	4	1
5	2	2	1
2	1	2	0
1	0	0	1
1	1	1	0
2	1	2	0
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2	0	2	1
3	1	0	1
2	2	0	0
1	1	3	0
0	0	1	0
0	3	1	2
2	0	3	1
0	0	1	2
0	0	0	1
1	1	1	3
0	1	0	1
0	0	0	0
0	1	0	0
0	1	0	1
0	1	0	0
0	1	0	0
0	0	1	0
1	0	0	0
1	0	0	0
1	0	0	0
0	0	0	0
1	0	2	1
1	0	1	0
0	1	0	1
0	0	0	0
0	0	0	1
0	0	1	0
1	1	1	1
0	0	0	1

0	1	0	1
1	0	0	0
0	0	0	0
0	0	1	0
0	0	0	0
1	0	1	1
0	0	0	0
0	0	0	2
1	0	0	0
0	0	0	0
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0	0	0	0
1	0	0	0
0	0	0	0
0	1	0	0
0	0	1	1
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0	0	1	0
0	0	0	1
0	0	0	0
1	0	0	0
2	0	0	0
1	0	1	1
0	1	0	0
0	0	0	1
0	0	2	0
0	0	0	0
0	1	0	0
0	0	0	0
1	0	2	0
1	0	0	1
0	0	0	0
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0	0	1	0
0	1	1	0
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0	0	1	0
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0	0	0	0
1	0	0	0
0	0	0	0
0	0	0	0
0	0	1	0
0	0	0	1
1	0	0	0
0	1	0	0
0	0	1	1
0	0	1	0
0	0	0	0
0	0	0	0
0	1	0	0
0	1	0	0
0	1	0	2
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