



TAMPERE UNIVERSITY OF TECHNOLOGY

# PATTERN RECOGNITION AND MACHINE LEARNING

Lecture 1: Introduction and the Basics of Python

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# Course Organization

- Organized on 3rd period; January – February 2017.
- Lectures every Tuesday 14-16 (TB111) and Friday 14-16 (TB111).
- 9 groups of exercises between Tuesday and Friday (sign up at POP).
- More details: <http://www.cs.tut.fi/courses/SGN-41007/>



# Course Requirements

- 1 60% of exercise assignments solved. For 70 %, you get 1 point added to exam score; for 80 % two points and for 90% three points.
- 2 Project assignment, which is organized in the form of a pattern recognition competition. The competition is done in groups.  
<https://inclass.kaggle.com/c/gene-expression-prediction>
- 3 Written exam. Max. number of points for the exam is 30 with the following scoring.

Points	<15	<18	<21	<24	<27	$\geq 27$
Grade	0	1	2	3	4	5



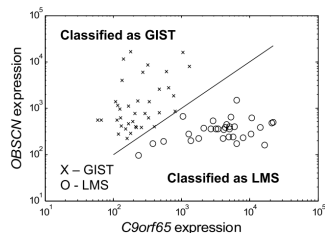
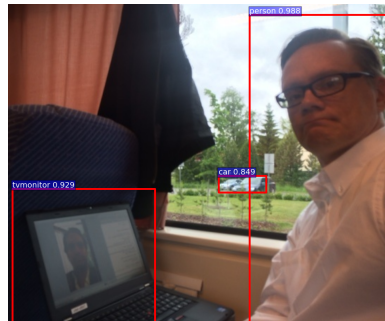
# Course Contents

- 1 **Python:** Rapidly becoming the default platform for practical machine learning
- 2 **Estimation of Signal Parameters:** What are the phase, amplitude and frequency of this noisy sinusoid
- 3 **Detection Theory:** Detect whether there is a specific signal present or not
- 4 **Performance evaluation:** Cross-Validation, Bootstrapping, Receiver Operating Characteristics, other Error Metrics
- 5 **Machine Learning Models:** Logistic Regression, Support Vector Machine, Random Forests, Deep Learning
- 6 **Avoid Overlearning and Solve Ill-Posed Problems:** Regularization Techniques



# Introduction

- Machine learning has become an important tool for multitude of scientific disciplines.
- Training based approaches are rapidly substituting traditional manually engineered pipelines.
- **Training based** = we show examples of what is interesting and hope the machine learns to do it for us
- **Model based** = we have derived a model of the data and wish to learn the unknown parameters
- A few modern research topics:
  - Image recognition (what is in this image and where?)
  - Speech recognition (what do I say?)
  - Medicine (data-driven diagnosis)



Price et al., "Highly accurate two-gene classifier for differentiating gastrointestinal stromal tumors and leiomyosarcomas," *PNAS* 2007.



# Why Python?

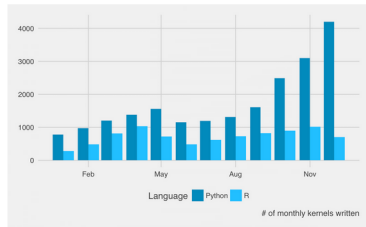
- Python is becoming increasingly central tool for data science.
- This was not always the case: 10 years ago everyone was using Matlab.
- However, due to licensing issues and heavy development of Python, scientific Python started to gain its user base.
- Python's strength is in its variability and huge community.
- There are 2 versions: Python 2.7 and 3.6. We'll use the former one as it's better supported by most packages interesting to us.

All Python releases are Open Source (see <http://www.opensource.org> for the Open Source Definition).

Historically, most, but not all, Python releases have also been GPL-compatible;

## Kernels & Datasets

R used to be the language of choice on Kaggle, but 2016 has seen Python emerge as a clear winner. Will Python maintain its constrictive grip in the coming year?



Source: Kaggle.com newsletter, Dec. 2016



# Alternatives to Python in Science

## Python vs. Matlab

- Matlab is #1 workhorse for linear algebra.
- Matlab is professionally maintained *product*.
- Some Matlab's toolboxes are great (Image Processing tb). Some are obsolete (Neural Network tb).
- New versions twice a year. Amount of novelty varies.
- Matlab is expensive for non-educational users.

## Python vs. R

- R has been #1 workhorse for statistics and data analysis. <sup>a</sup>
- R is great for specific data analysis and visualization needs.
- Lots of statistics community code in R.
- Python interfaces with other domains ranging from deep neural networks (Caffe, Theano) and image analysis (OpenCV) to even a fullblown webserver (Django/Flask)

<sup>a</sup> <http://tinyurl.com/jynezuq>

- "Matlab is made for mathematicians, R for statisticians and Python for programmers."



# Essential Modules

- **numpy**: The matrix / numerical analysis layer at the bottom
- **scipy**: Scientific computing utilities (linalg, FFT, signal/image processing...)
- **scikit-learn**: Machine learning (our focus here)
- **matplotlib**: Plotting and visualization
- **opencv**: Computer vision
- **pandas**: Data analysis
- **statsmodels**: Statistics in Python
- **caffe, theano, tensorflow, keras**: Deep neural networks (we are using keras later in the course)
- **spyder**: The front end (Scientific PYthon Development EnviRonment)





# Where to get Python?

- It is possible to construct your custom Python environment by installing individual modules (base from [python.org](https://python.org) and libraries from, e.g., <http://www.lfd.uci.edu/~gohlke/pythonlibs/>).
- Alternatively, one may install a full distribution, such as
  - Anaconda <https://www.continuum.io/downloads> ← **my favorite**
  - Enthought Canopy <http://www.enthought.com/>
- ...or in linux:

```
# apt-get install python
# apt-get install python-numpy
# apt-get install python-sklearn
# apt-get install python-matplotlib
# apt-get install spyder
```



# The Language

- Python was designed to be a highly readable language.
- Python uses whitespace to delimit program blocks. First you hate it, later you love it.
- All used modules are imported using an import declaration.
- The members of a module are referred using the dot: `np.cos([1,2,3])`
- Interpreted language. Also interactive with IPython extensions.

```
8 import matplotlib.pyplot as plt
9 import numpy as np
10 from sklearn.linear_model import Ridge
11 from sklearn.linear_model import Lasso
12
13 def get_obs_matrix(x, order = 5):
14     """
15     Return the observation matrix
16     constructed from powers of vector x.
17     """
18
19     H = []
20
21     for k in range(order):
22         H.append(x**k)
23
24     H = np.array(H).T
25
26     return H
27
28 if __name__ == "__main__":
29
30     # generate a noisy sinusoid
31
32     np.random.seed(2015)
33
34     x = np.arange(0,1.01,0.08)
35     y = np.cos(2 * 2*pi*x) \
36         + 0.35*np.random.randn(x.shape[0])
37     y2 = np.cos(1 * 2*pi*x) \
38         + 0.35*np.random.randn(x.shape[0])
39     x = np.arange(0,1.01,0.04)
```



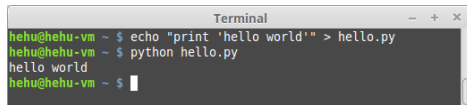
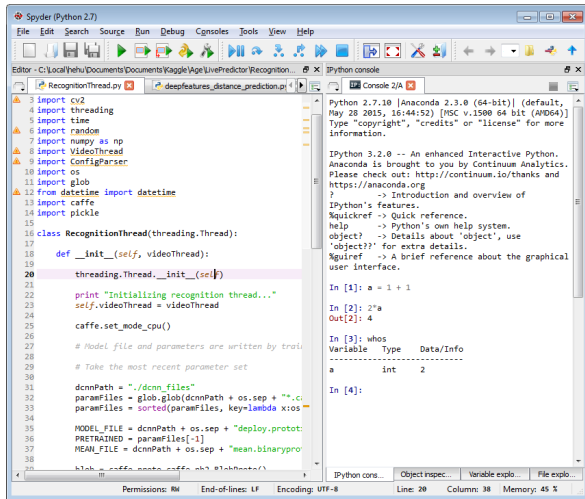
# Things to Come

- Following slides will introduce the basic Python usage within scientific computing.
  - **The editor and the environment**
    - *Matlab slightly better than Python*
  - **Linear algebra**
    - *Matlab better than Python*
  - **Programming constructs** (loops, classes, etc.)
    - *Python better than Matlab*
  - **Machine learning**
    - *Python a lot better than Matlab*



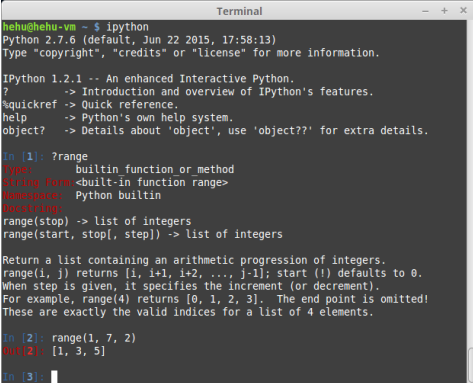
# Spyder Editor

- In this course we use the *Spyder* editor.
- The editor window contains two panes: editor on the left and console on the right.
- **F5**: Run code; **F9**: Run selected region.
- Alternatively, you can use whatever editor you like, and run everything on the command line.



# Python Basics

- Python code can be executed either from a script file (\*.py) or in the interactive mode (just like Matlab).
- For the interactive mode; just execute *python* from the command line.
- Alternatively, *ipython* (if installed) starts Python in a more user-friendly mode:
  - Tab-completion works
  - Many utility functions (e.g., `ls`, `pwd`, `cd`)
  - *Magic* functions (e.g., `%run`, `%timeit`, `%edit`, `%pastebin`)



```
Terminal
hehu@hehu-vm ~ $ ipython
Python 2.7.6 (default, Jun 22 2015, 17:58:13)
Type "copyright", "credits" or "license" for more information.

IPython 1.2.1 -- An enhanced Interactive Python.
?      -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help    -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.

In [1]: ?range
Type:      builtin function or method
String Form: <built-in function range>
Namespace: Python builtin
Docstring:
range(stop) -> list of integers
range(start, stop[, step]) -> list of integers

Return a list containing an arithmetic progression of integers.
range(i, j) returns [i, i+1, i+2, ..., j-1]; start (!) defaults to 0.
When step is given, it specifies the increment (or decrement).
For example, range(4) returns [0, 1, 2, 3]. The end point is omitted!
These are exactly the valid indices for a list of 4 elements.

In [2]: range(1, 7, 2)
Out[2]: [1, 3, 5]

In [3]:
```

*Command range creates a list of integers. Compare to Matlab's syntax 1:2:6.*



# Help

- For each command, help is there to refresh your memory:

```
>>> help("".strip) # strip is a member of the string class
Help on built-in function strip:

strip(...)
    S.strip([chars]) -> string or unicode

    Return a copy of the string S with leading and trailing
    whitespace removed.
    If chars is given and not None, remove characters in chars instead.
    If chars is unicode, S will be converted to unicode before stripping
```

- In *ipython*, the shortcut `?` is available, too (see previous slide).
- Many people prefer to Google for python `strip` instead; matter of taste.



# Using Modules

- Python libraries are called *modules*.
- Each module needs to be imported before use.
- Three common alternatives:
  - 1 Import the full module: `import numpy`
  - 2 Import selected functions from the module:  
`from numpy import array, sin, cos`
  - 3 Import all functions from the module:  
`from numpy import *`

```
>>> sin(pi)
NameError: name 'sin' is not defined
>>> from numpy import sin, pi
>>> sin(pi)
1.2246467991473532e-16
```

```
>>> import numpy as np
>>> np.sin(np.pi)
1.2246467991473532e-16
```

```
>>> from numpy import *
>>> sin(pi)
1.2246467991473532e-16
```



# Using Modules

A few things to note:

- All methods support shortcuts; e.g.,  
import numpy as np.
- Sometimes import <module> fails, if the module is in fact a collection of modules. For example, import scipy. Instead, use import scipy.signal
- Importing all functions from the module is not recommended, because different modules may contain functions with the same name.

```
>>> import scipy
>>> matfile = scipy.io.loadmat("myfile.mat")
AttributeError: 'module' object has no attribute 'io'
```

```
>>> import scipy.io as sio
>>> matfile = sio.loadmat("myfile.mat") # Works OK
```

```
>>> from scipy.io import loadmat
>>> matfile = loadmat("myfile.mat") # Works OK
```





# NumPy

- Practically all scientific computing in Python is based on numpy and scipy modules.
- NumPy provides a numerical array as an alternative to Python list.
- The list type is very generic and accepts any mixture of data types.
- Although practical for generic manipulation, it becomes inefficient in computing.
- Instead, the NumPy array is more limited and more focused on numerical computing.

```
# Python list accepts any data types
v = [1, 2, 3, "hello", None]
```

```
# We like to call numpy briefly "np"
>>> import numpy as np

# Define a numpy array (vector):
>>> v = np.array([1, 2, 3, 4])

# Note: the above actually casts a
# Python list into a numpy array.

# Resize into 2x2 matrix
>>> V = np.resize(v, (2, 2))

# Invert:
>>> np.linalg.inv(V)
array([[ -2. ,  1. ],
       [ 1.5, -0.5]])
```



# More on Vectors

- `np.arange` creates a range array (like `1:0.5:10` in Matlab)

```
>>> np.arange(1, 10, 0.5) # Arguments: (start, end, step)
array([ 1. ,  1.5,  2. ,  2.5,  3. ,  3.5,  4. ,  4.5,  5. ,  5.5,  6. ,
        6.5,  7. ,  7.5,  8. ,  8.5,  9. ,  9.5])

# Note that the endpoint is not included (unlike Matlab).
```

- Most vector/matrix functions are similar to Matlab:

```
>>> np.linspace(1, 10, 5) # Arguments: (start, end, num_items)
array([ 1. ,  3.25,  5.5 ,  7.75, 10. ])

>>> np.eye(3)
array([[ 1.,  0.,  0.],
       [ 0.,  1.,  0.],
       [ 0.,  0.,  1.]])

>>> np.random.randn(2, 3)
array([[ -2.23506417,  0.47311746,  0.05343861],
       [ 1.255074 , -0.03576461,  0.96121907]])
```



# Matrices

- A matrix is defined similarly; either by specifying the values manually, or using special functions.

```
# A matrix is simply an array of arrays
# May seem complicated at first, but is in fact
# nice for N-D arrays.

>>> np.array([[1, 2], [3, 4]])
array([[1, 2],
       [3, 4]])

>>> from scipy.linalg import toeplitz, hilbert # You could also " ...import *"
>>> toeplitz([3, 1, -2])
array([[ 3,  1, -2],
       [ 1,  3,  1],
       [-2,  1,  3]])

>>> hilbert(3)
array([[ 1.          ,  0.5          ,  0.33333333],
       [ 0.5        ,  0.33333333,  0.25       ],
       [ 0.33333333,  0.25        ,  0.2        ]])
```



# Matrix Product

- Matrix multiplication is different from Matlab. Use `np.dot` or `np.matmul`.
- With NumPy version 1.10+ and Python 3.5+, matrix multiplication can be done with the `@` operator: `A @ B`.

```
>>> A = np.array([[1, 2], [3, 4]])
>>> B = np.array([[5, 6], [7, 8]])

>>> A * B # Elementwise product (Matlab: A .* B)
array([[ 5, 12],
       [21, 32]])

>>> np.dot(A, B) # Matrix product; alternatively: np.matmul
array([[19, 22],
       [43, 50]])
```

```
$ python3
Python 3.5.2 (default, Nov 17 2016, 17:05:23)
>>> import numpy as np
>>> A = np.random.rand(3,3)
>>> B = np.random.rand(3,3)
>>> A @ B
array([[ 0.28382296,  0.90172558,  1.10036663],
       [ 0.39959554,  1.12141386,  1.39473854],
       [ 0.28797509,  0.82918235,  1.04229714]])
```



# Indexing

- Indexing of vectors uses the colon notation, too.
- Below, we extract selected items from the vector 1...10:

```
>>> x = np.arange(1, 11)
>>> x[0:8:2] # Unlike Matlab, indexing starts from 0
array([1, 3, 5, 7])

# Note: use square brackets for indexing
# Note2: colon operator has the order start:end:step;
# not start:step:end as in Matlab
```

- The start and end points can be omitted:

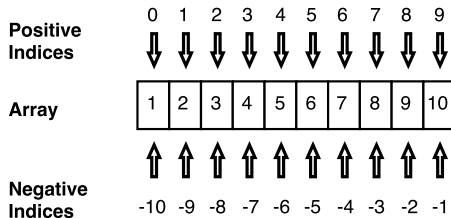
```
>>> x[5:] # All items from the 5'th
array([ 6,  7,  8,  9, 10])
>>> x[:5] # All items until the 5'th
array([1, 2, 3, 4, 5])
>>> x[::3] # All items with step 3
array([ 1,  4,  7, 10])
```



# Indexing

- Negative indices are counted from the end (-1 = the last, -2 = second-to-last, etc.):

```
>>> x[-3:] # Three last items  
array([ 8,  9, 10])  
>>> x[::-1] # Items in inverse order  
array([10,  9,  8,  7,  6,  5,  4,  3,  2,  1])
```



# Indexing

- Also matrices can be indexed similarly. This operation is called *slicing*, and the result is a *slice* of the matrix.
- Here we request for items on the rows 2:4 = [2,3] and columns 1,2,4 (shown in red).
- Note, that with matrices, the first index is the row; not "x-coordinate".
- This order is called "Fortran style" or "column major" while the alternative is "C style" or "row major".

```
>>> M = np.reshape(np.arange(0, 36), (6, 6))
array([[ 0,  1,  2,  3,  4,  5],
       [ 6,  7,  8,  9, 10, 11],
       [12, 13, 14, 15, 16, 17],
       [18, 19, 20, 21, 22, 23],
       [24, 25, 26, 27, 28, 29],
       [30, 31, 32, 33, 34, 35]])

>>> M[2:4, [1,2,4]]
array([[13, 14, 16],
       [19, 20, 22]])
```



# Indexing

- To specify only column or row indices, use ":" alone.
- Now we wish to extract two bottom rows.
- `M[4:, :]` reads "give me all rows after the 4th and all columns".
- In this case, alternative forms would be, *e.g.*, `M[-2:, :]` and `M[[4,5], :]`.

```
>>> M = np.reshape(np.arange(0, 36), (6, 6))
array([[ 0,  1,  2,  3,  4,  5],
       [ 6,  7,  8,  9, 10, 11],
       [12, 13, 14, 15, 16, 17],
       [18, 19, 20, 21, 22, 23],
       [24, 25, 26, 27, 28, 29],
       [30, 31, 32, 33, 34, 35]])

>>> M[4:, :]
array([[24, 25, 26, 27, 28, 29],
       [30, 31, 32, 33, 34, 35]])
```





# N-Dimensional arrays

- Higher-dimensional arrays are frequently encountered in machine learning.
- For example, a set of 1000 color images of size  $w \times h = 128 \times 96$  is represented as a  $1000 \times 3 \times 96 \times 128$  array.
- Here, dimensions are: image index, color channel, y-coordinate, x-coordinate.
- Sometimes, a shorter name is used: "(b, c, 0, 1) order".

```
# Generate a random "image" array:
>>> A = np.random.rand(1000, 3, 96, 128)

# What size is it?
>>> A.shape
(1000L, 3L, 96L, 128L)

# Access the pixel (4, 3) of 2nd color channel
# of the 2nd image
>>> A[1, 2, 3, 4]
0.36569219631994954

# Request all color channels:
>>> A[1, :, 3, 4]
array([ 0.32306666,  0.60012626,  0.3656922 ])
```

```
# Request a complete 96x128 color channel:
>>> A[1, 2, :, :]
array([[ 0.19102217 ...
        0.88464718]])

# Equivalent shorter notation:
>>> A[1, 2, ...]
array([[ 0.19102217 ...
        0.88464718]])
```



# Functions

- Functions are defined using the `def` keyword.
- Function definition can appear anywhere in the code.
- Functions can be imported to other files using `import`.
- Function arguments can be *positional* or *named* (see code).
- Named arguments improve readability and are handy for setting the last argument in a long list.

```
# Define our first function
def hello(target):
    print ("Hello " + target + "!")

>>> hello("world")
Hello world!

>>> hello("Finland")
Hello Finland!

# We can also define the default argument:
def hello(target = "world"):
    print ("Hello " + target + "!")

>>> hello()
Hello world!

>>> hello("Finland")
Hello Finland!

# One can also assign using the name:
>>> hello(target = "Finland")
Hello Finland!
```



# Loops and Stuff

```
for lang in ['Assembler', 'Python', "Matlab", 'C++']:
    if lang in ["Assembler", "C++"]:
        print ("I am ok with %s." % (lang))
    else:
        print ("I love %s." % (lang))
```

```
I am ok with Assembler.
I love Python.
I love Matlab.
I am ok with C++.
```

```
# Read all lines of a file until the end
```

```
fp = open("myfile.txt", "r")
lines = []
```

```
while True:
```

```
    try:
```

```
        line = fp.readline()
        lines.append(line)
```

```
    except:
```

```
        # File ended
        break
```

```
fp.close()
```

- Loops and other usual programming constructs are easy to remember.
- for can loop over anything *iterable*, such as a list or a file.
- In Matlab, appending values to a vector in a loop is not recommended. Python lists are actual lists, so appending is fine.



# Example: Reading in a Data File

- Suppose we need to read a csv file (text file with Comma Separated Values) into Python.

```
1 Sample_ID,M1;M2;M3;M4;M5;M6;M7;M8;M9;M10;M11;M12;M1
2 S0;0.063915;0.033242;0.018484;0.0086177;0.035629;0.
3 S1;0.025409;0.051085;0.056305;0.021738;0.02741;0.01
4 S2;0.025536;0.036123;0.054195;0.009735;0.027521;0.0
5 S3;0.012817;0.029652;0.07929;0.050677;0.039737;0.05
6 S4;0.019846;-0.010577;-0.0075045;0.019042;0.068786;
```

- The file consists of 216 rows (samples) with 4000 measurements each.
- We will write file reading code from scratch.
- Alternatively, many modules contain csv-reading functions
  - `numpy.loadtxt` or `numpy.genfromtxt`
  - `csv.reader`
  - `pandas.read_csv`



# Example: Reading in a Data File

```
import numpy as np

if __name__ == "__main__":

    X = [] # Rows of the file go here

    # We use Python's with statement.
    # Then we do not have to worry
    # about closing it.

    with open("ovarian.csv", "r") as fp:

        # File is iterable, so we can
        # read it directly (instead of
        # using readline).

        for line in fp:

            # Skip the first line:
            if "Sample_ID" in line:
                continue
```

```
        # Otherwise, split the line
        # to numbers:
        values = line.split(";")

        # Omit the first item
        # ("S1" or similar):
        values = values[1:]

        # Cast each item from
        # string to float:
        values = [float(v) for v in values]

        # Append to X
        X.append(values)

    # Now, X is a list of lists. Cast to
    # Numpy array:
    X = np.array(X)

    print ("All data read.")
    print ("Result size is %s" % (str(X.shape)))
```



# Visualization

```
import matplotlib.pyplot as plt
import numpy as np

N = 100
n = np.arange(N) # Vector [0,1,2,...,N-1]
x = np.cos(2 * np.pi * n * 0.03)
x_noisy = x + 0.2 * np.random.randn(N)

fig = plt.figure(figsize = [10,5])

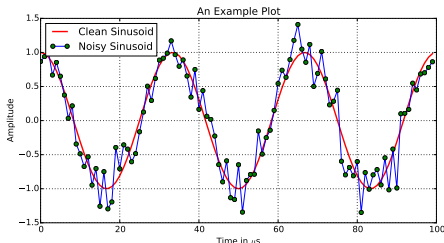
plt.plot(n, x, 'r-',
         linewidth = 2,
         label = "Clean Sinusoid")

plt.plot(n, x_noisy, 'bo-',
         markerfacecolor = "green",
         label = "Noisy Sinusoid")

plt.grid("on")
plt.xlabel("Time in  $\mu$ s")
plt.ylabel("Amplitude")
plt.title("An Example Plot")
plt.legend(loc = "upper left")

plt.show()
plt.savefig("../images/sinusoid.pdf",
            bbox_inches = "tight")
```

- The matplotlib module is our plotting library.
- Function names are often similar to Matlab.
- Usually you want to "import matplotlib.pyplot".
- Alternatively, "from matplotlib.pyplot import \*" makes the environment very similar to Matlab.
- Code also in <https://github.com/mahehu/SGN-41007>



# Another Example

- Even rather complicated graphics are easy to generate using Matplotlib.
- The code for the attached diagram is shown in <https://github.com/mahehu/SGN-41007>.

