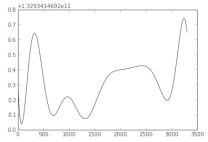
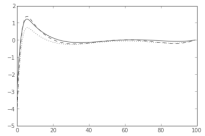
```
>>> import ni
>>> data = ni.data.monkey.Data(condition = 0)
>>> model = ni.model.ip.Model({'cell':4,'crosshistory':[6,7]})
>>> fm = model.fit(data.trial(range(data.nr_trials/2)))
>>> plot(fm.prototypes()['rate'],'k')
```



```
>>> with ni.figure("",close=False):
        plot(fm.prototypes()['autohistory'],'k-')
        plot(fm.prototypes()['crosshistory6'],'k--')
        plot(fm.prototypes()['crosshistory7'],'k:')
```



Bootstrapping Information Criterion for Stochastic Models of Point Processes

&

The **ni.** Python Toolbox

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Contents

Versicherung an Eides statt

Hiermit erkläre ich diese Masterarbeit selbständig verfasst und nur die angegebenen Quellen und Hilfsmittel verwendet zu haben.

Chapter 1

Introduction

This thesis presents a toolbox for modeling neuronal activity in the framework of statistical models. A process of *model selection* is discussed, using the Extended Information Criterion (EIC) to obtain a way of comparing models of varying complexity.

Chapter 2 will introduce a model that can be used to predict neural activity using a Generalized Linear Model (GLM) and separate components to model rate, autohistory and interactions with other cells. Chapter 3 refreshes some concepts used in the Python programming language, such that chapter 4 can introduce the **ni.** toolbox and how it implements the model of chapter 2 (Section 4.3.1), represents data (Section 4.2) and provides tools for the utilization of the IKW computing grid and result presentation (Section 4.4). Chapter 5 then illustrates how to perform model selection using the toolbox and how the bootstrapped information criterion compares to less computationaly intense measures such as Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC) (introduced in 5.0.7 and 5.0.8).

1.1 Comparing Models

For neuronal activity, prediction is no goal in itself, as it is eg. for weather models. Rather, how good a model matches the actual activity gives insight into the process behind the activity. When two models are compared, the one that matches the data more closely can be considered as more representative for the physical process. The structural differences between the models, such as an interaction between two certain cell assemblies,can then be interpreted as structural features of the physical process. But when data is finite, the problem of over-fitting and the problem of biased estimators arise.

1.1.1 The Problem of Over-Fitting

When only a finite amount of data is used to fit a model, the model has to extract characteristics from the data and interpolate how further data samples might look like. A model that is more complex than the process behind the data tends to infer behavior in the data that in actuality is never found because, as the model is fitted, it will adapt to noise in the data more effectively than a simple model. A term that was supposed to model an interaction between two cells now models the interaction of one of those cells and a very specific instance of noise fluctuations. By modeling the noise, the complex model can achieve a closer fit to the training data, but it will have problems predicting new data, as the noise is not a part of the modeled process and therefore not present in the new data.

Such a model is said to have over-fitted. It tried to match the training data as accurately as possible, and in doing so it missed the essential characteristics of the process that it could have found in other instances of data.

1.1.2 The Problem of Bias

When a model is evaluated in how close it can predict data it was trained on, an over-fitting model will (by defintion) always score better than a simpler, but more representative model. The likelihood is *biased* - it will systematically be estimated higher than it actually is on unseen data. So not only is a complex model bad at predicting future data, it also overestimates its ability to do so.

But evaluating a model by comparing it to newly acquired data is difficult. Take eg. the case of electrode recordings: the relative position to cell assemblies and changes by neural plasticity or the physical insertion of the electrodes can change the recorded activity in such a way that the previous model no longer applies to new recordings that are taken some weeks after the first. Thus, a split of the data of one recording session into a part that is used for training and a part that is used for fitting is the most common method to evaluate models and perform a *model selection*. Some models use model selection in their own fitting process. This requires additional splits of the data into quarters, eights, sixteenths, etc.

It would be much more practical if one could use the data one has to acquire anyway to fit the model to also evaluate the model. To accomplish this, the bias of the likelihood has to be estimated and compensated for to obtain an unbiased *information criterion*, which judges how well a model explains the data.

As the bias tends to scale with complexity, one method to do this is to subtract a penalty for each used parameter in the model. The AIC (see Section 5.0.7) builds on this principle. However, the bias is different on different data statistics, which is why [Ishiguro et al., 1997] proposed a bias correction that uses the bootstrapping method to simulate data fluctuations. This method is discussed in section 5.0.9 and in chapter 5 the **ni** python toolbox will be used to build a number of models, to compare them and to infer connectivity hypotheses solely on the basis of evaluations using training data, which are then compared

to evaluations using previously unseen data.

1.1.3 Toolbox

The toolbox can be obtained from: `https://github.com/jahuth/ni/`

The documentation is available at: `http://jahuth.github.io/ni/index.html` and additional information on how to use the toolbox is in the appendix of this thesis.

Chapter 2

The GLM Pointprocess model

2.1 Definition of a Model

A model is a mapping from *parameters* into a probability distribution on *features*. The direction from parameters to features is called a *prediction*, the inverse mapping, from features to parameters, is called the *fit*.

How good a model matches a physical process can be measured by comparing the prediction with the actual data, yielding a *likelihood* of the data, given the model.

One goal of modeling would be to infer facts about the world from the parameters of the model that describes the data best. If a parameter in a model makes it believable that some interaction between two neurons is taking place, one would like to think that this interaction is actually plausible.

To find out whether the parameters actually represent hidden qualities of the data, one can evaluate the model by cross evaluation, ie. fitting on some part of the data and predicting the remaining part.

2.2

The goal of the models discussed in this thesis is to predict the firing probability of a cell assembly at some time t dependent on the previous time steps of the same and other assemblies, using model components that each model a part of the probability:

$$p(x(t) = 1|x(t_{t-1}), \dots x(t_0)) = \sum_i \cdot p_i \left(x(t) = 1|x(t-1), \dots x(1), x(0)\right) \quad (2.1)$$

2.3 Notations

To make indexing parts of a spike train easier, we use a notation that selects a range of values between two indices, including the first, but excluding the last index:

$$x_{[a:b]} := \begin{cases} x(a), x(a+1), \dots x(b-1) & \text{if } a > b \\ x(a), x(a-1), \dots x(b+1) & if b > a \\ x(a) & else \end{cases} \tag{2.2}$$

The vector $x_{[a:b]}$ is therefore $|b-a|$ elements long.

The set of spikes up to a timepoint t will be denoted as:

$$S_t := \{\tau | x(\tau) = 1 \text{ and } \tau < t\} \tag{2.3}$$

With this notation Equation 2.1 becomes:

$$p(x(t) = 1 | x_{[t:0]}) = \prod_i \cdot p_i(x(t) = 1 | x_{[t:0]}) \tag{2.4}$$

2.4 Generalized Linear Models

To now model the probability with a Generalized Linear Model (GLM), we rewrite 2.4 using some functions f_i and a link function g as:

$$p(x(t) = 1 | x_{[t:0]}) = g^{-1}\left(\sum_i \beta_i \cdot f_i(x_{[t:0]})\right) \tag{2.5}$$

g is a link function, f_i are arbitrary functions and β_i are coefficients. The linear combination of the weighted functions, scaled by the link function, is used to model the probability of a spike for each time point t.

The β_i coefficients are what is to be optimized in the fitting process of the GLM. The index i runs over a set of functions that can be grouped into *Components* that each model a certain aspect of the spike train.

To predict a Bernoulli distribution, g should be the *logit* function, which is the inverse of the logistic function (see Figure 2.4.1 and Equation 2.7). The logistic function maps the real line into an interval between 0 and 1, such that probabilities can be represented as arbitrarily large values. The larger a value is, the closer the probability is to 1. The more negative it is, the closer the probability is to 0. A value of 0 translates to a 0.5 probability.

$$logit(p) = log(p) - log(1-p) \tag{2.6}$$

$$logit^{-1}(x) = \frac{1}{1+e^{-x}} \tag{2.7}$$

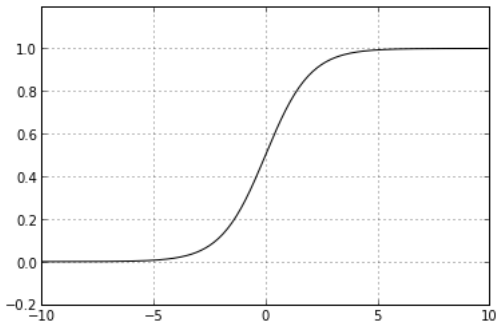


Figure 2.4.1: The logistic function, which is used to map values into probabilities. The logit function (the inverse of the logistic function) is used to map probabilities to values.

2.5 Properties of Spike Trains

Spike trains can be written as a sum of Dirac δ functions:

$$\rho(t) = \sum_{i=1}^{n} \delta(t - t_i)$$

t_i is spike number i, n being the number of spikes. See also [Dayan and Abbott, 2001]

The Dirac δ function is defined on a discrete timeline[1] at time t as:

$$\delta(t) = \begin{cases} 1 & \text{for } t = 0 \\ 0 & else \end{cases}$$

The function $\rho(t)$ will be zero almost everywhere, except at the time points that contain a spike. An integral over a portion of this function will yield the number of spikes in this portion.

2.5.1 The Sifting Property

A Dirac δ function has the property of selecting a value from a function when applied in an integral or sum:

$$\int d\tau \delta(t - \tau) h(\tau) = h(t)$$

Which means, that if a kernel is multiplied with a spike train, the kernel can be thought of as being filtered at each spike for its value. If a kernel is folded

[1] On the real numbers the definition differs, but this does not need to concern us as we only use discrete time.

on a spike train, the reverse kernel is appended to each spike. A kernel that is defined on negative values ("looking into the past") will project the influence of the spike forward in time.

This means that if we want to calculate the influence on some time t by some spikes and a kernel, it is equivalent to express the influence as Equation 2.8 as a sum over time-points or 2.9 as a sum over the set of spikes. Since there are less spikes than time points, the second method results in less computation.

$$f(t) = \sum_{\tau} x(t-\tau) \cdot kernel(\tau) \tag{2.8}$$

$$f(t) = \sum_{s \in S} kernel(s-t) \tag{2.9}$$

The following code illustrates the two formulas:

```
import scipy
spikes = np.zeros(1000)
for i in rand(10) * 1000:
    spikes[int(i)] = 1
kernel = np.zeros(100)
kernel[70] = 1
kernel = scipy.ndimage.gaussian_filter(kernel,10)
# first method:
out = np.zeros(1100)
for t in range(1100):
    out[t] = 0
    for tau in range(100):
        if (t-tau) >= 0 and (t-tau) < 1000:
            out[t] = out[t] + (spikes[t-tau] * kernel[tau])
# second method
out2 = np.zeros(1100)
for t in where(spikes)[0]:
    out2[t:(t+100)] = out2[t:(t+100)] + kernel
```

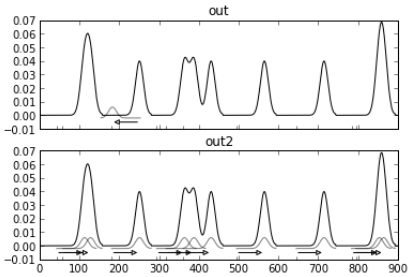


Figure 2.5.1: Using the sifting property, spike influence can be calculated in O(spikes), rather than O(timesteps): The first method computes the sum of the kerneled spikes for every time point (looking back), the second method adds up time shifted kernels (looking forward in time). Both methods are equivalent.

2.6 Splines

To utilize the linear combination of functions in the GLM to model smooth time series, these time series are approximated as *splines*, made up of a linear combination of basis splines (b-splines). They are written as a small, bold **b** in this text, with a lower index signifying that a certain basis spline out of a set is considered. The number of basis splines in a set is referred to as k.

The basis splines in the FMTP [Costa, 2013] code and hence the **ni.** toolbox are created recursively with the formulas (originally implemented by Niklas Wilming for the NBP eye-tracking toolbox):

$$B_{j,1}(x) := \begin{cases} 1 & \text{if } x \text{ lies between the knots } j \text{ and } j+1 \\ 0 & else \end{cases} \tag{2.10}$$

and to calculate b-splines of an order k:

$$B_{i,k}(x) := \frac{x - t_i}{t_{i+k} - t_i} \cdot B_{i,k-1}(x) + \frac{t_{i+k} - x}{t_{i+k} - t_{i+1}} \cdot B_{i+k,k-1}(x) \tag{2.11}$$

To compute basis spline i of order k at point x, the recursive formula computes a weighted average between the lower order splines of this and the k-next index, weighted by the relative distance to each of the knots.

2.7 Rate Model

To model rate fluctuations that are similar across all trials (or a subset, ie. all trials with a certain condition), a spline function is spanned over the entire trial duration, being separated in k basis splines.

$$f_{rate}(t) = b_0 + \sum_{i=1}^{k} \beta_i \mathbf{b}_i(t) \tag{2.12}$$

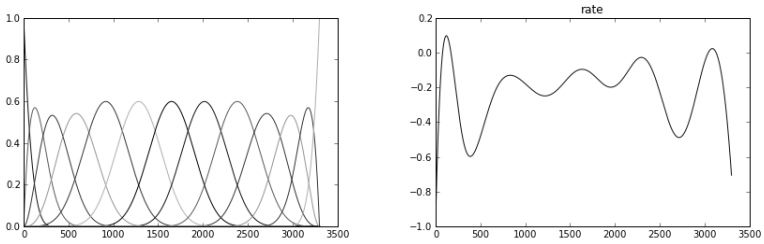


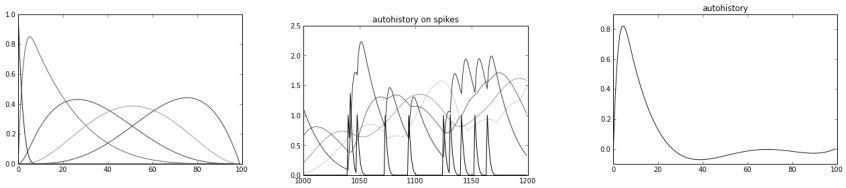
Figure 2.7.1: A set of rate basis splines and an example of a fitted spline.

2.8 First Order History

Since spikes are also dependent on the activity of other regions and its own history, it makes sense to model this term relative to the current time bin. We should assume, that events in the very distant past are negligible in relation to recent events and model only a time interval between t and $t-m$, with m being the length of memory that is assumed. If one argues that the further a spike is in the past, the less important its exact location becomes, one should use a logarithmic spaced spline function to model this, if one disagrees, a regular spline spacing is also possible.

$$f_{history}(x_{[t:0]}) = b_0 + \sum_{i=1}^{k} \beta_i \mathbf{b}_i^T x_{[t:t-m]} \tag{2.13}$$

This history term can be used without modification on other spike trains, such that it models $p(x_a = 1 | x_{b[t:0]})$



(a) (b) (c)

Figure 2.8.1: (a) a set of history basis splines, (b) the components folded on a spike train and (c) an example of a fitted spline.

2.9 Higher Order History

The first order history term has the fault that a fine grained placement of spikes (eg. in bursting activity) is averaged into a single history term. To differentiate behavior in high firing rate regimes and low firing rate regimes, one needs to include more than one spike at a time in the model.

Taking spikes at two distances i and j in the spike train past, we would want to model interactions that influence the current bin as:

$$f_{2nd\ history}(x_{[0:t]}) = \sum_{i=1}^{m} \sum_{j=1}^{m} h(i,j) x(t-j) x(t-i) \tag{2.14}$$

$h(i,j)$ models the interactions of spikes at time $t-i$ and $t-j$. The term $x(t-j)x(t-i)$ selects an value out of the h matrix at entry i,j.

If we assume $h(i, j)$ not to be arbitrary and sparse, but rather a smooth surface, we have to use splines again to fit this surface to the few data points we have:

$$h(i,j) = \sum_{i_1=1}^{k_1} \sum_{i_2=1}^{k_2} \beta_{i_1,i_2} \mathbf{b}_{i_1}(i) \mathbf{b}_{i_2}(j) \tag{2.15}$$

m being the memory length of the history component, k_1 being the number of splines in the first set, k_2 the number in the second.

Following [Schumacher et al., 2012], the coefficients can be taken out of the multiplication of spike trains, such that the spike trains folded with each basis spline can be multiplied with each of the other folded spike trains to get each component across the complete trial interval.

$$f_{2nd\ history}(x_{[0:t]}) = \sum_{i_1=1}^{k_1} \sum_{i_2=1}^{k_2} \beta_{i_1,i_2} \left(\sum_{i=1}^{m} \mathbf{b}_{i_1}(i) \cdot x(t-i) \right) \cdot \left(\sum_{j=1}^{m} \mathbf{b}_{i_2}(j) \cdot x(t-j) \right) \tag{2.16}$$

Because of symmetry the term in the sum of j in Equation 2.15 can be restricted to $j > i$, if we use the same basis functions for every dimension. Then, however, we can no longer isolate $\left(\sum_{j>i}^{m} \mathbf{b}_{i_2}(j) \cdot x(t-j) \right)$ as a single term, since it would then depend on i.

But using the symmetry for the case of using the same basis splines, the number of coefficients can be reduced, as the coefficient $\beta_{a,b}$ will have the same independent variables as $\beta_{b,a}$, since the same spikes are concerned. This would result in $\beta_{a,b}$ and $\beta_{b,a}$ adding up to the actual interaction coefficient $\beta_{a,b+b,a}$. So $\beta_{b,a}$ can be set to 0 for all $b > a$ to reduce the (apparent) model complexity:

$$f_{2nd\ history}(x_{[t:0]}) = \sum_{i_1=1}^{k_1} \sum_{i_2 \geq i_1}^{k_2} \beta_{i_1,i_2} \left(\sum_{i=1}^{m} \mathbf{b}_{i_1}(i) \cdot x(t-i) \right) \cdot \left(\sum_{j=1}^{m} \mathbf{b}_{i_2}(j) \cdot x(t-j) \right) \tag{2.17}$$

m being the memory length of the history component, k_1 being the number of splines in the first set $\mathbf{b}_{i_1}$, k_2 the number in the second set $\mathbf{b}_{i_2}$. The coefficients β_{i_1,i_2} will be re-indexed in the model.

The model component implementing this part of the model will be discussed in Section 4.3.2.5.

2.10 How the Components are Used in the Model

The standard model provided by the **ni.** toolbox is a combination of a rate model, an autohistory model and a crosshistory model for each cell in the data. Additional parts can be added to the model by editing the **Configuration** of the model (eg. a higher order autohistory term). To fit the model, or to predict data, a design matrix is constructed using these **Component**s (see Section 4.3.2) and spike data, calculating $f_{c_i}(t)$ for $t \in [0 \dots T]$ and all parts of all components c_i.

The resulting matrix is then used to calculate the optimal coefficients β_i to maximize the likelihood of Equation 2.5 using one of the statistical modeling python libraries (see Section 4.3.1.2).

Since the model uses the linear combination of the single model components f_{c_i}, the formulas of this section are always used as a given, fixed time series - whether fitting or predicting. They are calculated once from a set of spikes, creating a series of values. Afterwards the mathematical definition of each component is no longer considered in the fitting or prediction process. The only exception is when spikes are generated from an existent model (see Section 4.3.3) in the case of first order history components. To make computation easier, rather than re-calculating the complete $f_{autohistory}$ component whenever a spike is set, the fitted spline function of the autohistory component is added to the rate function, essentially adding up to the definition in Equation 2.13.

Chapter 3

Python for Scientific Computations

Python is a programming language developed for code readability and (relative) platform independence. It is an interpreted language as it is not translated into architecture-dependent machine code, but run inside an interpreter. Computationally expensive operations can be handled by platform specifically compiled libraries written in C or Assembler.

The **scipy** project[1], including the packages **matplotlib**, **numpy**, **scikit** (and many more) and the interactive **iPython** console, enable python to be useful for scientific computations, such as large scale data analysis and visualization, statistical modeling and even symbolic mathematics[2].

Python uses indentation levels to indicate program flow. Variables are loosely typed and can contain different types at different time points. Lists and dictionaries are built-in types that can save an array of variables, indexed with a number for lists or indexed by a string for dictionaries.

Python packages are organized in *modules* (see Section 3.1). Modules, classes and functions are named as described in Section 3.2. *Exceptions* and *Context Managers* are two concepts used in the toolbox that make code more readable and act reasonable in case of errors. Sections 3.3 and 3.4 give a short introduction to these concepts. Source code is only useful when properly documented. The **sphinx** package can create html documentation from python code as described in 3.5.

A local *git* repository has been used for private version control and to publish code easily to the IKW servers. The release version is published on github: `https://github.com/jahuth/ni/` along with the documentation at `http://jahuth.github.io/ni/index.html`

[1] `http://www.scipy.org/`

[2] `http://www.sympygamma.com/input/?i=limit%28x*log%28x%29%2C+x%2C+0%29`

3.1 Python Modules

Python provides object oriented programming mechanisms that make it easy to encapsulate code such that it does not interfere with other parts of the program. Classes and functions can be part of a *module* (in the simplest case a .py file) that can be *included* in programs and provides a save name space for these classes and functions.

The **ni.** toolbox is a module that includes other modules for easy access. They are grouped in three sub-modules **ni.data.**, **ni.model.** and **ni.tools.** which in turn contain the modules for data representation, modeling and miscellaneous tasks respectively.

When a module is included in a script, it is compiled to python byte-code, which means that the module only needs to be parsed once by the python parser and - if no changes are made to the module - can be accessed almost as fast as a binary library.

3.2 Naming Convention

Based loosely on [van Rossum et al., 2001], the following conventions were followed for naming:

- All lowercase for modules: **module**. Underscores may be used to improve readability as in **ni.tools.html_view**.
- Class names are **CamelCase**, starting with a capital letter and starting each new word with a capital letter with no underscores, colons, etc. separating words.
- Functions and methods are named **all_lower_case_with_underscores** or **camelCaseStartingWithLowerLetter**, arguments of functions and methods are named similarly. If a verb as a name for a function is modified in the text of this thesis, only the actual name of the function is **print**ed as a keyword.
- A leading underscore is used to signify that an attribute is `_hidden`
- module wide constants are all `CAPITAL_LETTERS`, words separated by underscores.

3.3 Exceptions in Python

Contrary to most languages, exceptions in python are expected to come up. They even are preferred to return values such as `False`, `0` or `-1` for unsuccessful function calls (if eg. a file can not be opened). If an exception is not handled by an **except:** block, it will be raised to the user, showing a backtrace of what lead to the exception. Still, exceptions should only be handled for specific cases

and seldom with a catch-all, except for code that runs in a sandbox or contains user written code.

An example for how exceptions are used as a language feature is the following:

```
x1 = randint(10)
x2 = randint(10)
y = randint(10)
if (x1-x2) != 0:
    ratio = y/(x1-x2)
else:
    ratio = y
```

```
x1 = randint(10)
x2 = randint(10)
y = randint(10)
try:
    ratio = y/(x1-x2)
except ZeroDivisionError:
    ratio = y
```

When code in a **try:** block fails, the **except** `Handler:` block is asked to handle the exception. If no handler matches the exception, it is raised further. If one were to signal a non-existent file or some inconsistent arguments in some innermost function code using return codes such as `False`, `0`, `-1`, or even predefined constants, every function that uses some code that could fail and fails with it, would have its return value checked whether something went wrong. Exceptions bypass all of this, straight to the code that actually knows what to do in case of non-existent files or inconsistent arguments.

Using **if**-statements before calling a potentially failing function would not always result in a manageable amount of checks and can interfere with encapsulation of object oriented programming, making it harder to exchange code that has basically the same functionality, but eg. lacks some limitations (one example would be to go from a text-file based logging mechanism to a database). With exceptions, deprecated limits do not need to be checked.

In the toolbox, exceptions are mostly raised as the default **Exception** type, but using a custom messages like `"End of Jobs"`.

3.4 Context Managers

A nice way that python uses to make writing code more easy are so called Context Managers, which are objects that contain an __**enter**__ and an __**exit**__ method (surrounded by two underscores). The most common example is the built-in **file** type:

```
with open("a_master_thesis.txt", "w+") as f:
    f.write("Some text.")
```

The function **open** returns a **file** object, which is also a Context Manager. Instead of properly opening the file and closing it after writing to it is done, the file is opened as soon as the context is entered. The indented code can access the object under the name **f** and after the code is completed, the file is closed.

This is useful to improve the readability of ploting code. An example of normal **matplotlib** plotting code would be:

```
fig = pylab.figure()
for (x,y) in data_1:
    plot(x,y)
title("Important Data")
fig_2 = pylab.figure()
for (x,y) in data_2:
    plot(x,y)
title("Other Data")
fig.savefig("plot_1.png")
fig_2.savefig("plot_2.png")
```

Similarly to matlab and R, the default **matplotlib** method is to save **figure** handles in variables, while the active figure is remembered by the plotting library and follows a stacking behavior: first-in, last-out. If one remembers the handle, a previous figure can be activated at a later point, while the stack structure remains intact.

The code can be rewritten to use Context Managers from the **ni.** toolbox:

```
with ni.View("results.html") as view:
    with view.figure("plot_1.png"):
        for (x,y) in data_1:
            plot(x,y)
        with view.figure("plot_1.png"):
            for (x,y) in data_2:
                plot(x,y)
            title("Other Data")
        title("Important Data")
```

Even if in this example no care was given to structure the code in terms of which figure is plotted into at which time, the indentation makes it clear which plot function call corresponds to which active figure. Since each figure is closed at the **__exit__** call, the stack behavior is made explicit.[3]

This mechanism becomes useful particularly in the case of **Exceptions** (see Section 3.3). If some code within the **with** block fails, the **__exit__** method will still be called and also informed that an error took place so that files can be closed and data can be cleaned up. Normally, figures would remain opened, disturbing further code, clogging up memory and preventing partially finished figures to be written to files. A Context Manager will close the figures and write them to a file.

Classes in the toolbox that act as context managers are:

- **ni.Figure**, provided by the function **ni.figure(`filename`)**, saves a figure as if called via **pylab.figure()** and **pylab.savefig(`filename`)**. Additionally, the figure is closed unless **ni.figure** has been called with `close=False`, in which case the previously active figure will be activated again.

- **ni.tools.html_view.Figure**, provided by the **.figure(`path`)** method of the **View** class saves a figure into the **View** object it was called from. The figure will be transformed into a base 64 encoded string, such that it can be included in an html file.

[3] Of course there can be use cases where this behavior is detrimental to the flow of computation or memory usage. Figure handles can still be used.

- The **View** class itself, if instantiated with a filename, renders the output to the specified location.

3.5 Documentation

Python code should always be documented with doc-strings for every module, class and function. Doc-strings are an integral part of the language and are actually present whenever a function is used:

```
print ni.data.data.merge.__doc__
```

The iPython notebook and console provide the doc string as a tooltip and the sphinx documentation package[4] generates comprehensive html or pdf documentation from *re-structured text (ReST)* doc strings. The **ni.** toolbox documentation is available on `http://jahuth.github.io/ni/index.html`

Below, the first lines of the **data** module python file show an example of a doc string that is compiled into the documentation (see Figure 3.5.1).

```
"""
.. module:: ni.data.data
   :platform: Unix
   :synopsis: Storing Point Process Data

.. moduleauthor:: Jacob Huth

.. todo::
        Use different internal representations, depending on use. Ie. Spike times vs. binary array

.. todo::
        Lazy loading and prevention from data duplicates where unnecessary. See also: 'indexing view versus
              copy <http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-view-versus-copy>'_

Storing Spike Data in Python with Pandas
----------------------------------------------------------

The 'pandas package <http://pandas.pydata.org/>'_ allows for easy storage of large data objects in python.
       The structure that is used by this toolbox is the pandas :py:class:'pandas.MultiIndexedFrame' which is
       a :py:class:'pandas.DataFrame' / 'pandas.DataFrame <http://pandas.pydata.org/pandas-docs/dev/dsintro.
       html#dataframe>'_ with an Index that has multiple levels.

The index contains at least the levels ''Cell'', ''Trial'' and ''Condition''. Additional Indizex can be
        used (eg. ''Bootstrap Sample'' for Bootstrap Samples), but keep in mind that when fitting a model
       only ''Cell'' and ''Trial'' should remain, all other dimensions will be collapsed as more sets of
       Trials which may be indistinguishable after the fit.


==========  =====  ======= ================================
Condition    Cell   Trial   *t* (Timeseries of specific trial)
==========  =====  ======= ================================
0            0      0       0,0,0,0,1,0,0,0,0,1,0...
0            0      1       0,0,0,1,0,0,0,0,1,0,0...
0            0      2       0,0,1,0,1,0,0,1,0,1,0...
0            1      0       0,0,0,1,0,0,0,0,0,0,0...
0            1      1       0,0,0,0,0,1,0,0,0,1,0...
...          ...    ...     ...
1            0      0       0,0,1,0,0,0,0,0,0,0,1...
1            0      1       0,0,0,0,0,1,0,1,0,0,0...
...          ...    ...     ...
==========  =====  ======= ================================


To put your own data into a :py:class:'pandas.DataFrame', so it can be used by the models in this toolbox
       create a MultiIndex for example like this::

    import ni
    import pandas as pd
    d = []
    tuples = []
    for con in range(nr_conditions):
"""
```

[4] `http://sphinx-doc.org/`

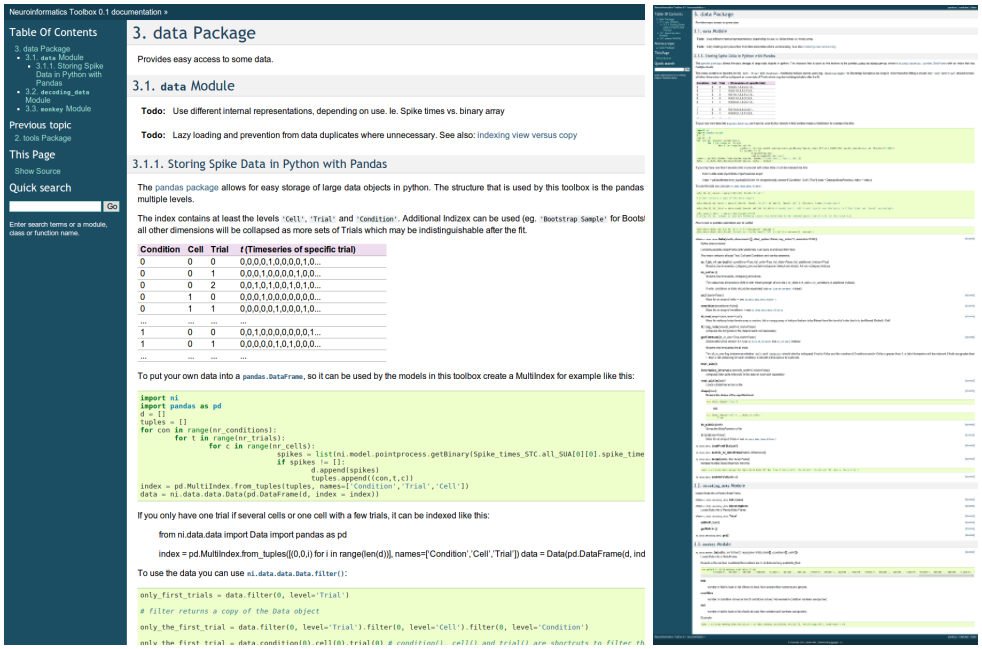


Figure 3.5.1: A sphinx documentation page

Chapter 4

Modules of the `ni.` Toolbox

4.1 ni.config - Toolbox Configuration Options

Some variables have default values for the complete toolbox. To give the user control over these variables, the **ni.config** saves and loads these variables from the files: `ni_default_config.json`, `ni_system_config.json` and `ni_user_config.json`. The default configuration file is part of the toolbox and should not be altered, except when the changes are submitted back to the toolbox repository. The system configuration file contains default changes that can be made by administrators or course advisors and the user configuration file should contain all preferences that only apply to the specific user.

For every option that is requested by the toolbox, first the user option is used, if it exists. If it does not exist, the system option is used, if it is not set in the system file either, the default value is used. However, code using the **config** module should still have a default value ready, in case the default configuration file is missing the specific option as well.

Configuration options can be changed directly in the files, if the json syntax is maintained, or alternatively by calling `ni.config.user.set(option, value)` and subsequently `ni.config.user.save()`

Using the options in the code is done by requesting an option with `ni.config.get(option, default_value)`.

To request all set options in all config files, `ni.config.keys(True)`, lists them in the order of over-ride. To get a list of only unique option names, the python type **set** [1] can be used: `set(ni.config.keys(True))`

[1] as in set theory, not as a verb

4.2 Providing Data: the ni.data Modules

4.2.1 ni.data.data - a Common Structure

Spike data can be organized via the **Data** class. It contains a Pandas MultiFrame, which contains rows of trials, indexed with Trial, Cell, Condition and possible additional indices.

Pandas **DataFrame**s are similar to DataFrames used in R (see eg. `http://stat.ethz.ch/R-manual/R-devel/library/base/html/data.frame.html`). DataFrames store data (eg. time series) of equal length. It is indexed two-dimensionally and behaves very similar to two-dimensional matrices. But it can also contain meta data to index entries in the DataFrame more elaborately. For pandas specifically, a DataFrame can be thought of as an indexed collection of **Series**, which are in some ways equivalent to **numpy ndarray**s.

A **DataFrame** can be build from a dictionary of **Series**, or from an unlabeled matrix. To use a Hierarchical Index (**MultiIndex**), the index has to be created such that it corresponds to the single entries in the **DataFrame**.

The following code demonstrates how to convert a 3d-indexed set of spike time lists into a multi-indexed DataFrame:

```
from ni.model.pointprocess import getBinary
d = []
index_tuples = []
for condition in range(self.nr_conditions):
    for trial in range(self.nr_trials):
        for cell in range(self.nr_cells):
            d.append(list(getBinary(spike_times[condition,trial,cell
                ].flatten()*resolution)))
            index_tuples.append((condition,trial,cell))
index = pandas.MultiIndex.from_tuples(index_tuples, names=['
    Condition','Trial','Cell'])
data = pandas.DataFrame(d, index = index)
```

An example to use data from eg. the **nltk** toolkit would be to define points on different channels as the occurrence of letters. This means eg. to have one channel for word separators and one for one of the vowels *a*, *e*, *i* each and to take different languages as conditions. To use this setup with the toolbox, models simply convert the occurrences to binary arrays and add them to a list, with an index tuple at the same position in the index list.

```
import ni
import numpy as np
import pandas
from nltk.corpus import genesis
from ni.model.pointprocess import getBinary
trial_length = 1000 # use blocks of this many characters as a trial
d = []
index_tuples = []
for (condition, txt_file) in enumerate(['english-kjv.txt','finnish.
    txt','german.txt','french.txt']):
    s = genesis.raw(txt_file).replace('.\n',' ').replace('\n',' ').
        replace('.',' ') # to make the end of sentences also ends of
         words
```

```
    for t in range(len(s)/trial_length):
        for (cell, letter) in enumerate([' ', 'a', 'e', 'i']):
            d.append(list(getBinary( np.cumsum([len(w)+1 for w in s
                [(t*trial_length):((t+1)*trial_length)].split(letter
                )]) )))
            index_tuples.append((condition,t,cell))
index = pandas.MultiIndex.from_tuples(index_tuples, names=['
    Condition','Trial','Cell'])
data = ni.Data(pandas.DataFrame(d, index = index))

model = ni.model.ip.Model({'history_length':10, 'rate':False})
for condition in range(4):
    fm = model.fit(data.condition(condition).trial(range(50)))
    print str(condition)+': ' + ' '.join([str(fm.compare(data.
        condition(i).trial(range(50,100)))['ll']) for i in range(4)
        ])
```

Figure 4.2.1 shows spike plots for one trial. The likelihoods of the models trained on each of the conditions will print as something like:

```
0: -363.370063515 -547.122975071 -381.937801005 -454.057645381
1: -503.786012045 -381.38280323  -432.132176101 -476.044628726
2: -392.585078922 -492.461953592 -354.180694395 -453.905837921
3: -400.67833968  -446.436570567 -387.665897328 -400.7340132
```

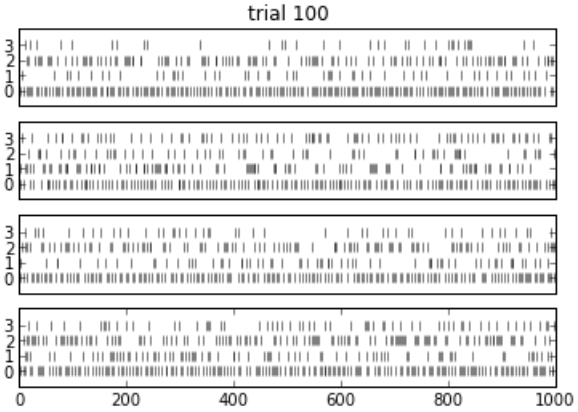


Figure 4.2.1: Using a few lines of code, data from other python toolkits like the **nltk** can be used as pointprocess data. This plot shows one block of data counting occurrences of word separators and the vowels a, e and i (as channels 0 to 3) in the (subplots from top to bottom) English, Finnish, German and French version of the genesis corpus of the **nltk**.

Another example on how to create an actual data module can be found in the appendix.

4.2.2 ni.data.monkey

For this module to work, the **`ni.data.monkey.path`** variable of the **config** module has to be set to a directory containing the `.mat` files of the data from [Gerhard et al., 2011] as provided to me by Gordon Pipa. This directory should be accessible by the user and - if possible - from any machine in the IKW network eg. on a network storage. While this module is mostly an example, other spike data can be provided similarly in their own modules.

Using this data set (or any other that provides its own module) should be as easy as:

```
import ni
ni.config.user.set("ni.data.monkey.path",
                   "/home/user/Data/Gerhard2011b")
data = ni.data.monkey.Data() # loads the first datafile
data.condition(0).cell([0,2,3]).trial(range(10)) # selects the first
     ten trials of cells 0, 2 and 3 of condition 0
```

Or if the dataset offers additional parameters:

```
import ni
import random
trial_number = random.choice(ni.data.monkey.available_trials)
data = ni.data.monkey.Data(trial_number,condition=0,cell=[0,2,3],
    trial=range(10))
    # loads a specific data file and only loads the specified trials
        , cells and condition
```

4.3 Providing Models: the ni.model Modules

4.3.1 .ip - Inhomogeneous Pointprocess Standard Model

A generalized linear model is a more flexible form of regression that uses a link function to predict the value of a target function. In the case of spike trains, this target function is 0 or 1, which means that 100% prediction is near to impossible and the best one can do is to get the prediction function as low as possible when there are no spikes and as high as plausible for when a spike is predicted.

If one takes the firing probability as a mean of a very large ensemble of neurons, the prediction tries to accurately match the percentage of firing neurons at any given time.

The model that is used for this toolbox contains methods to create a design matrix, fit the model via the **statsmodels.api.GLM** [Perktold et al., 2013] class, using the **statsmodels.genmod.families.family.Binomial** family to provide a link function, or the **sklearn.linear_model.ElasticNet** [scikit-learn developers, 2013]

To create a model, a **Configuration** instance or a dictionary containing configuration values is needed. Otherwise the default values are used.

Some important values are:

value	default	description
cell (int)	0	The number of the dependent cell
autohistory (bool)	`True`	Whether to include an autohistory component
crosshistory (bool or list)	`True`	Whether to include crosshistory components
rate (bool)	`True`	Whether to include a rate component
knots_rate (int)	10	Number of knots in the rate components
knots_number (int)	3	Number of knots in the history components
history_length (int)	100	Length of the history components
backend `"glm"` or `"elasticnet"`	`"glm"`	Which backend to use

Table 4.1: Configuration values of the **ip** Model. A full description can be seen in the documentation.

4.3.1.1 Generating a Design Matrix

Once the model is created, it can be used to **.fit** to data and **.save** itself to a text file. Also it can **.compare** a predicted time series to point process data using the appropriate functions.

In the **Model.fit** method, the dependent time series is extracted from the data and a design matrix is created from the configuration values and the data that is to be fitted to. The design matrix can also be obtained by the **Model.dm** method, the dependent time series by the **Model.x** method.

The design matrix is created by creating a **DesignMatrixTemplate** (see Section 4.3.2) and adding a number of components to it (a HistoryComponent on the dependent cell if `autohistory` is `True`, etc.). After all components are added, the Template is **combine**d with the data into an actual matrix, folding the history kernels onto spikes, adding the rate splines once every trial etc..

The finished design matrix is then inspected for rows that are only 0. The coefficients for these rows are set to zero.

4.3.1.2 Model Backends

When the **.fit** method of the selected backend is called, it chooses the coefficients, such that the the likelihood of $g^{-1}(Y \cdot \beta)$ on the time series x is maximal [2]. For the `"glm"` backend this is done by the `GLM` function with an Binomial Family object:

```
binomial_family = statsmodels.api.families.Binomial()
statsmodels.api.GLM(endog, exog, family=binomial_family)
```

with `endog` being the time series to predict and `exog` being the design matrix.

The `"elasticnet"` backend uses either the **sklearn.linear_model.ElasticNetCV()** to choose the regularization parameters by cross evaluation when the confguration option `crossvalidation` is set to `True`. Alternatively it uses the class **sklearn.linear_model.ElasticNet()** that uses an `alpha` and an `l1_ratio` value set in the configuration.

[2] Y is the design matrix/independent variables, β the coefficients and x the independent time series

4.3.1.3 Results of the Fit

After the fit is complete, the results are saved in a **FittedModel**. This object contains a reference to the model, the fitted coefficients as `.beta` and a range of statistic values, as provided by the chosen backend. A **FittedModel** can be **.save**d to a file, **.predict** other data and **.compare** the prediction to the actual data using the methods provided by the model class. Also it can return a dictionary of the fitted components added up to one *prototype* each.

4.3.2 .designmatrix - Data-independent Independent Variables

The **ni.model.designmatrix** module provides a class **DesignMatrixTemplate** that stores design matrix **Component**s. These components create rows for the actual design matrix when provided with data. As some components may require nontrivial computation on the data (eg. higher order spike dependencies) and the design matrix has to be computed completely from scratch for every prediction, rather than the actual design matrix only the components are saved in the model.

Rather than the actual design matrix, the model only remembers the template that was used to create the matrix. Since the design matrix is used at most twice, but can become very large as it has dimensions of the trial duration $\times$ the number of trials $\times$ the number of independent variables (ie. rows), a huge amount of memory is used up unnecessarily, if a large number of models is fitted for eg. bootstrapping or simple model comparison. Also the template is necessary to create new design matrices for predicting other data.

4.3.2.1 Constant and Custom Components

Components that are added to the design matrix should be derived from the class **designmatrix.Component** to make sure they contain all necessary methods to function as a design matrix component. Also the bare **Component** class can be used to insert arbitrary values into the design matrix.

The most trivial of all components is a *constant* that has to be added to all models and just provides a means of shifting all other components by arbitrary amounts. It is sufficient to only add a single 1 as a kernel (using `numpy.zeros((1,1))` to make sure it is a two dimensional 1), as the kernel will be repeated until the end of the time series.

When adding other time series as a kernel it should be noted that the correct orientation is used when adding the kernel to the component. The first dimension should align with the time bins (eg. be equal to the trial length), the second dimension holds different parts of the component, eg. different basis splines.

To have one component trying to cover firing rate trends over multiple trials one could write:

```
import ni
```

```
data = ni.data.monkey.Data(condition=0)
long_kernel = ni.model.create_splines.create_splines_linspace(data.
    nr_trials * data.trial_length,5,False)
ni.model.ip.Model({'custom_components': [ ni.model.designmatrix.
    Component(header='trend', kernel=long_kernel) ]})
```

4.3.2.2 Rate

A **Rate** component tries to model regular fluctuations of the firing rate that is the same in all trials.[3] This could be eg. the response to an experimental stimulus. It is important to keep in mind that if this stimulus is not at exactly the same point in time for all trials, one must rather encode the stimulus as an additional spike train and use a crosshistory component to fit the response.

The normal rate component is the sum of a number of linearly spaced splines that cover the whole trial duration. Each spline corresponds to a section of trial time and will be scaled to the mean firing rate at that point (taking into account other components as well). The sum of those splines gives a smooth function, no matter how the individual splines are scaled.

RateComponents can be configured with the `knots_rate` option. The length of the component is fixed to the trial length, but if a custom kernel is supplied, the length is not checked. The DesignMatrix will revert to the default behavior and concatenated the kernel on itself to fill the timeseries.

4.3.2.3 Adaptive Rate

If one suspects that some points in time require a higher resolution of modeling - which is usually the case if there is a fluctuation of firing rate - one can use a custom spacing of spline knots. The **AdaptiveRate** component will accept custom spacings, but - if non is provided - will also compute a spacing that will cover roughly the same number of spikes in each spline. Regions with higher firing rate will have a higher resolution, thus the model is more sensitive to firing rate changes, if the firing rate is high. Information theoretically this makes sense, as a low firing rate is harder to predict than a higher firing rate (as in a Poisson process, the variance scales with the firing rate), thus it should be smoothed more to prevent over fitting. A high firing rate allows very fine variations to be caught, which justifies a high resolution.

4.3.2.4 Autohistory and Crosshistory

To model how a neuron assembly regulates its own firing rate, eg. by a refractory period or self inhibition, one can use Equation 2.13 from Section 2.8 in a **HistoryComponent** that is set to the same spike train that it predicts.

A **HistoryComponent** requires as arguments the cell it is based on as a number (the `channel`), a length of memory (`history_length`), the number of knots to span a logarithmic spline function (`knot_number`) and a boolean value

[3] see Section 2.7 for the mathematical definition

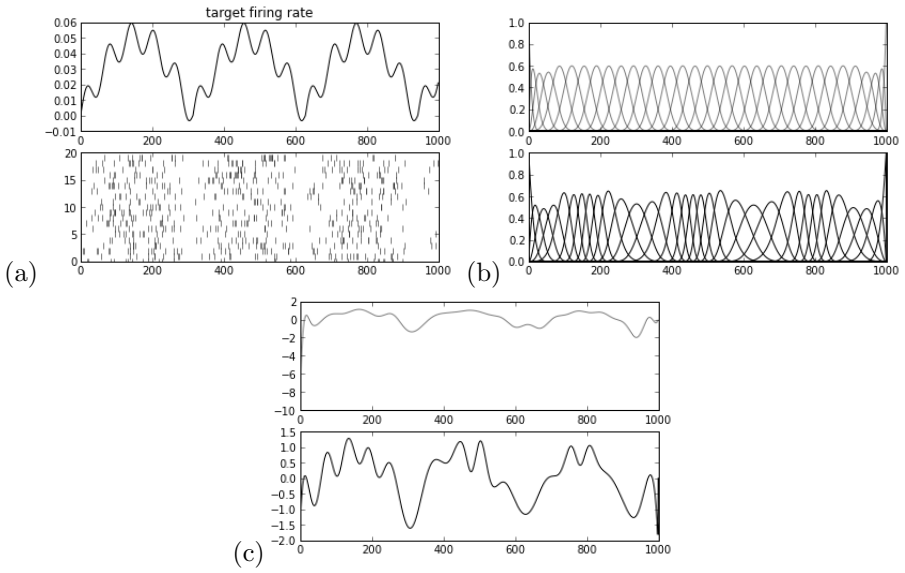


Figure 4.3.1: To model a rate function that has varying degrees of firing rate such as (a), it might make sense to use a higher resolution on the sections of the spike train that have a higher firing rate. (b) shows a comparison between linear knot spacing and adaptive knot spacing, taking into account the firing rate. (c) shows the resulting fitted rate functions: the grey lin-spaced rate function can't imitate the finer structures of the target. The black adaptive rate spaced function does a better job with the same number of basis splines. Tweaking the number of knots and the smooth-ness of the rate function used for the component, a close fit is possible.

whether the last basis spline should be omitted. Alternatively, one can supply the HistoryComponent with a ready made kernel as produced by the **create_splines_logspace** or **create_splines_linspace** helper functions in the **ni.model.create_splines** module.

The default values for the automatically created auto- and crosshistory components is taken from the model configuration. Also the flags for which history is to be considered are included in the configuration. The `autohistory` option can either be `True` or `False`, while the `crosshistory` option can contain a list of cell numbers that are to be used for history components.

4.3.2.5 2nd Order History Kernels

Higher order kernels, made up out of products of splines can be seen as the sum of products of one dimensional basis splines as discussed in Section 2.9

The prototype of this component are not two fitted spline functions, but a $k \times k$ matrix relating spikes at time i_1 and i_2 to a specific firing rate probability. However the matrix is not symmetric, as presumed by the definition, but

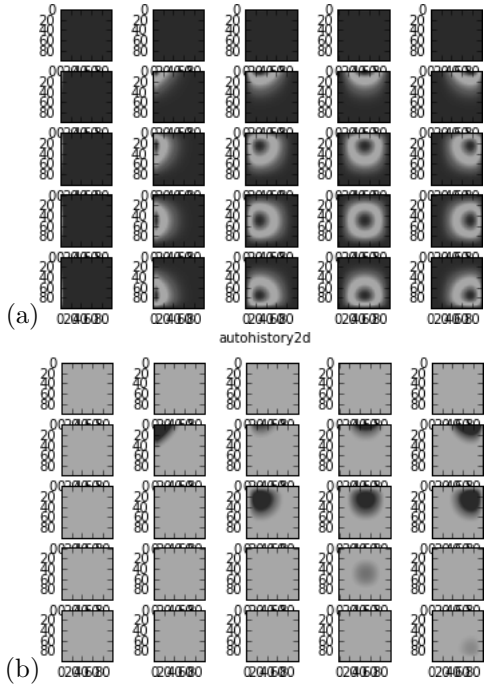


Figure 4.3.2: An example of a higher order history. (a) all combinations of basis splines (b) the fitted component only uses the upper half of the diagonal (including the diagonal combinations). Note that each matrix has some non-negative values below its diagonal.

assumes an arbitrary order ($i_1 < i_2$ or $i_2 < i_1$ pose no difference here). The b-spline combinations for the lower diagonal were omitted, as they are equal to the upper half. There are still some values below the diagonal non-zero, but this is caused by the b-splines not ending at the diagonal. Hence the actual value is not h_{i_1,i_2}, but rather $h_{i_1,i_2} + h_{i_2,i_1}$.

This may seem as if the symmetry is unused, but as the symmetry was actually used to reduce the number of coefficients, and the complexity trick of Section 2.9 only works for non-ordered spikes, this was the most plausible course of action.

4.3.3 .ip_generator - Turning Models back into Spike Trains

To generate new spikes from a model, one can use the fitted components to estimate a firing probability. This probability has to be scaled via the link function to get an actual probability, which can then be instantiated by a coin toss of exactly that probability for each bin.

In the simple rate-model case, this will generate a spike train that mimics the mean firing rates for every bin. If autohistory or crosshistory models are

used to generate spikes, the corresponding firing rate deviations are dependent on whether there was a spike in the past, ie. it depends on the coin tosses of the previous bins. This means, that on every coin toss, that created a spike, the history kernel has to be projected into future bins to modify the firing rate probability.

For higher dimensional history kernels, the probability is determined by the actual component on the basis of the previous spikes and kept separate from the firing rate that is modified by the first order history.

The current implementation only works with the standard design components, ie. a **RateComponent**, a **Component** named `'constant'`, optionally auto- and cross **HistoryComponent**s and higher order autohistory. If custom components are added, the generator needs to be extended to include these components, otherwise the generated spikes will deviate from the model severely.

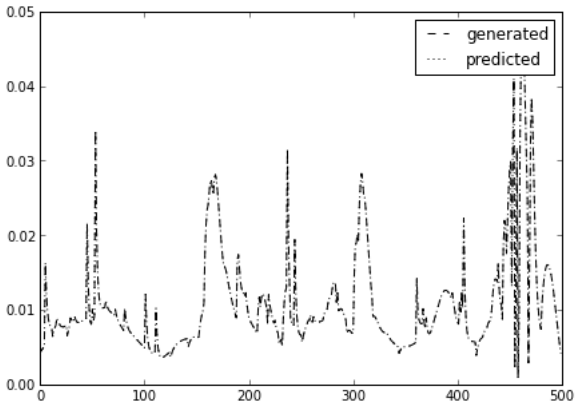


Figure 4.3.3: An example of created and predicted firing rates to test whether the **ip_generator** is functioning correctly.

A demo project illustrates, whether an implementation of a generator is correct. It fits models on some random data and then generates a new trial. Then the models are used to predict firing rate of the new trial. Since the generator not only returns the spike times, but also the firing probability that was used to generate the spikes, the firing rate probability can be compared. Since the probability for the generator and the model only depends on the past, the actual spikes that are generated are not important for their respective time bins. Therefore the probabilities should match perfectly - give or take only a numerical error[4].

4.3.4 .net_sim - A Generative Model

Another method to generate spike trains is to simulate a small network, very similar to **ip_generator**, but with a randomly generated connectivity. Only a

[4]Which for me was about 10^{-15} of maximal difference of the two functions

few connections are used and randomly assigned to be inhibitory or excitatory exponentially decaying influence kernels. The firing rate is constant for each neuron, and drawn randomly from the interval [0.4,0.6].

The module contains a function to simulate such a network, which returns a **SimulationResult** object. Also a class is available, which instantiates a random network in its constructor, providing the possibility to run the same network multiple times.

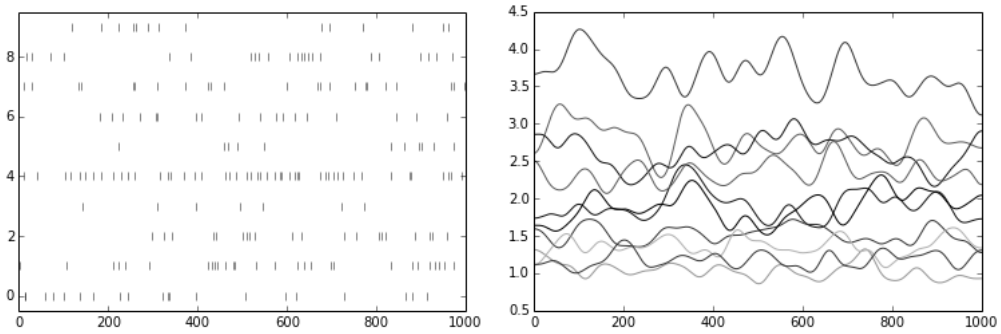


Figure 4.3.4: Example of a trial of spike data generated by the **net_sim** module.

4.3.5 .pointprocess - Collection of Pointprocess Tools

The **pointprocess** module collects functions that aid in the analysis of point processes. It provides a simple **PointProcess** container class, which holds a spike train in a sparse format. **createPoisson** creates a spike train from a firing rate or firing rate function p. Two functions convert between binary time series and lists of spike times: **getCounts** and **getBinary**. From binary representations, interspike intervals and from two spike trains a reverse correlation can be computed. A **SimpleFiringRateModel** class is supposed to act as a fast placeholder for model evaluations, using only the mean firing rate. However as the model only has one parameter, it is not a very interesting case.

4.4 Tools ni.tools

4.4.1 .pickler - Reading and Writing Arbitrary Objects

Python provides a method to save data structures to files. This method is called *pickling*, as in preserving them in a pickle jar.

The **ni.** toolbox **Pickler** class enables objects to be saved to and loaded from text files, either in *json* or *tab indented* format. Classes that inherit from **Pickler** have **.save** and **.load** methods, as well as a super constructor that can load from a dictionary of variables or string.

Pythons own **pickle** functionality can save the most common data structures. However it is not suitable to save objects that include references to other objects.

Further the aim of this module is to produce human readable and writable output with an easy to use syntax, such that models can be specified in text files rather than in running instances of programs.

A short example for a readable model file would be:

```
<class 'ni.model.ip.Model'>:
    configuration:
        <class 'ni.model.ip.Configuration'>:
            history_length:
                90
            knot_number:
                4
```

Further goals of this module is to be integrated with Robert Costas method of writing xml[Costa, 2013] and also to keep the generated code as short as possible by excluding the standard values, such that only the changes made to the standard configuration is saved. This however could also lead to problems if the standard values change.

4.4.2 .bootstrap - Calculating EIC

The bootstrap module aims to provide easy functions to calculate the bootstrap information criteria EIC. It takes a model, some original data and either bootstrap data or it trial shuffles the original data. Further it can calculate the performance of the bootstrap models on a range of test data. Three different functions can be used to calculate the bootstrap information criterion:

When data is generated from **Model** instances, **bootstrap_samples** will use one set of this data each as a bootstrap sample. It accepts a list of **ni.Data** instances, or a **ni.Data** instances containing an additional key `'Bootstrap Sample'`.

bootstrap_trials and **bootstrap_time** use the original data and re-draw from the set of trials or time points a comparable bootstrap sample. Figure 4.4.1 shows how this results in different design matrices.

The functions all return a dictionary containing the EIC, AIC, etc. and also the single EIC values for each bootstrap sample under the key `EICE` (for EIC-Estimates). This dictionary can be simply added to a **StatCollector**.

4.4.3 .project - Project Management

The **project** module provides tools to load python code and setting directories such that a script can be run multiple times and the output is created in a new directory. An instance of a running script and its Further it provides logging functions and preserves the variables in case of uncaught Exceptions. Also a code file can be split up into jobs.

The **frontend.py** program provides a *curses* user interface to projects and allows for monitoring and submitting of jobs to eg. the IKW grid, but it can also be used locally to queue jobs and run a small number of jobs in parallel.

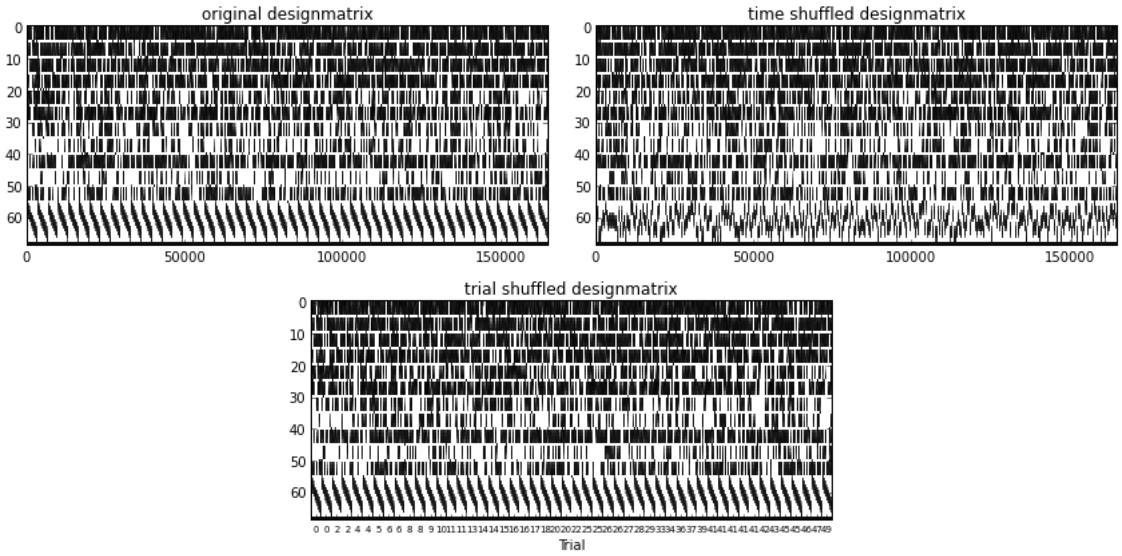


Figure 4.4.1: When using **bootstrap_trials** or **bootstrap_time**, the original data is re-drawn either from trial blocks or the complete design matrix is drawn from the set of time-points.

4.4.3.1 Parallelization

The statistical method of bootstrapping is possible because large-scale calculations have become reasonably cheap. Computations are especially easy, when there is a lot of independent tasks that can be done in parallel, even on completely different machines. Bootstrapping is such a task, as a large number of models are fitted on data that is previously available.

The IKW offers a computing grid to use resources on IKW computers effectively.[5]

The **ni.tools.project** module provides a relatively basic form of job parallelization. Unlinke the method developed by [Costa, 2013], which takes a callable and produces Grid jobs from it, this module parses the uncompiled source code and looks for **job ... :** statements. The code is then split up and a **Session** is created containing **Job** instances with each its own source code and dependencies.

A **job** statement is a line that starts with the keyword **job**, followed by a job name. This name should be unique within the file. Afterwards a number of **for** `var` **in** `list` pairs can create batches of this job, where each job has `var` set to one element of `list`. If multiple **for** statements occur, the crossproduct of the lists is used to generate jobs. Should this not be desired, **zip** should be used to combine two lists into one list of tuples with one element from the first, the second from the second list. The **job** statement has to end with a colon

[5] See: `https://doc.ikw.uni-osnabrueck.de/howto/grid`

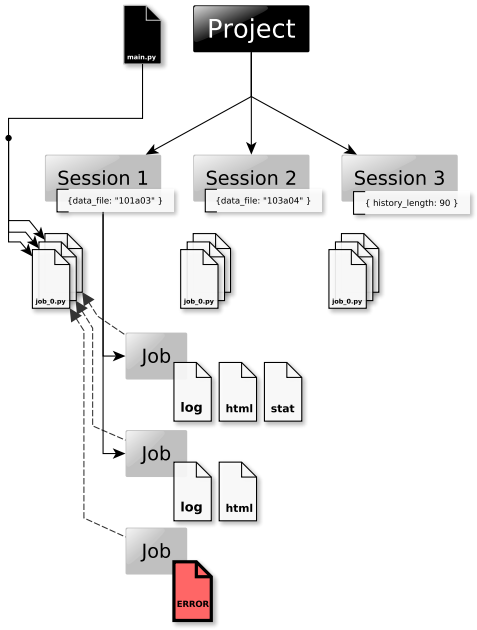


Figure 4.4.2: A **Project** can manage several sessions of the same task (eg. with some parameters changed). Each **Session** can contain several jobs from a python file containing job statements. This file is parsed into several job script files.

character ":". Code that should be part of the job has to be indented after the job statement. When the indentation level is lost again, following code will no longer be part of this job.

```
""" An example job file that will generate 110 jobs. """
## Parameters:
cells = range(10)
## End of Parameters
job "Printing a cell" for cell in cells:
    print cell
job "Printing more cells" for cell_1 in cells for cell_2 in cells:
    requires previous   # only do this if the previous job is
        completed
    print cell_1, cell_2
```

The block between the `## Parameters` and `## End of Parameters` comments can be edited on a per-session basis and saved as a text file `'parameters.txt'` into the session directory and will be replaced in the source code. It can also be passed as an argument to the function parsing the source file into job files.

An example use case of setting up a session with new jobs would be:

```
import ni
p = ni.tools.project.load("TestProject")
```

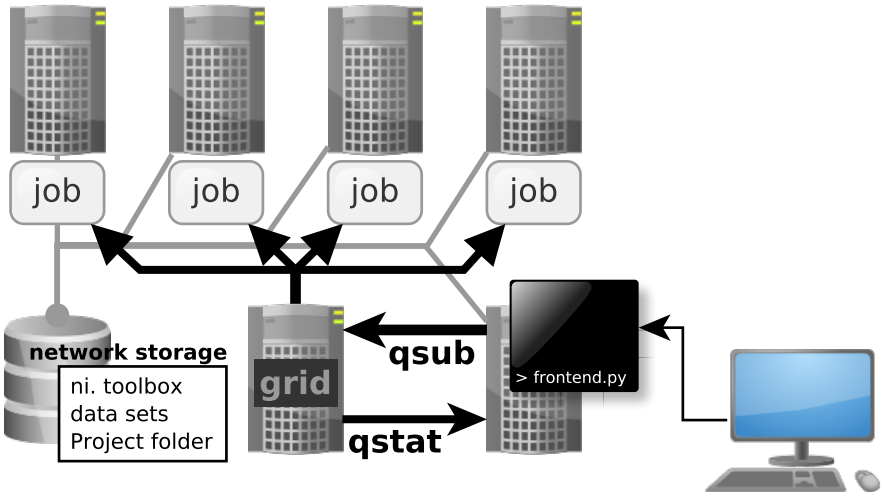


Figure 4.4.3: Using the grid with the ni. toolbox can be done via the `frontend.py` running on one of the university computers. The `frontend` program submits jobs to the grid controller and checks the status of the submitted jobs. If an option is set, it will update a html report every so often.

```
parameters = p.get_parameters_from_job_file()
parameters = parameters.replace("cells = range(10)","cells = [3,5,7]
    ")
p.create_session()
p.session.setup_jobs(parameter_string = parameters)
    # session refers to the currently active session for this
        project instance
```

A **Project** instance detects on initialization which **Session**s are present and what the status of each session is.

A number of helper programs make the handling with **Project**s easier:

- The **autorun.py** script submits grid jobs for all (or a specified number) of jobs until all jobs are done.
- The **frontend.py** script provides a **curses** UI to view projects and check on the progress of sessions. A screenshot is shown in Figure 4.4.4.
- The **ni.tools.html_view** module is capable of producing a html representation of a **Project**, **Session** or **Job**, which can also be updated automatically from **frontend.py**

Figure 4.4.4: The curses UI `frontend.py`: The project overview shows which jobs are running, which are pending and which are done. New sessions can be created from the command prompt within the frontend.

4.4.4 .plot - Plot Functions

4.4.4.1 plotGaussed

plotGaussed just plots a time series after convolving it with a gauss kernel to make eg. firing rates apparent in a spike plot.

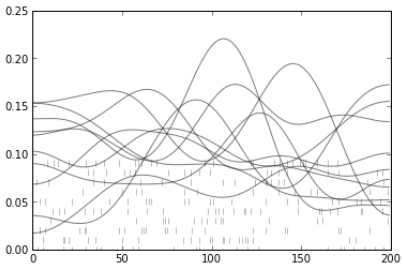


Figure 4.4.5: Smoothed spike trains produced with **ni.tools.plot.plotGaussed** show the mean firing rate

4.4.4.2 plotHist

To plot smoothed histograms **plotHist** adds up gaussian bell curves of a specific width. The mean of the distribution is marked on the line and depending on the smoothness of the distribution, it may or may not coincide with the peak of a gauss curve.

4.4.4.3 plotNetwork and plotConnections

To visualize connections between cell assemblies, these two functions either draw a connection matrix or a network graph.

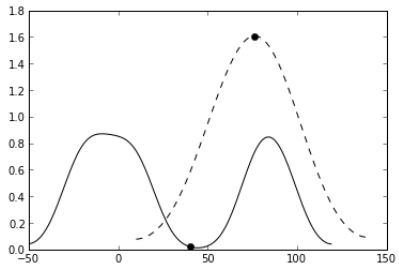


Figure 4.4.6: Two smooth histograms of a unimodal and a bimodal distribution as shown with **ni.tools.plot.plotHist**.

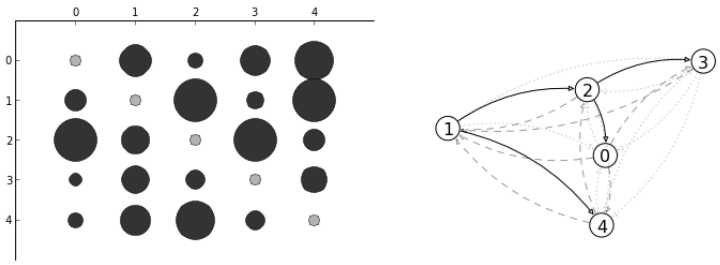


Figure 4.4.7: Visualizations of a random network as a connection matrix and as a graph.

The graph visualization requires **networkx** to be installed and normalizes the weights to the maximum value for each row (or column, depending on the options set). This forces at least one incoming edge per node and is the default setting since likelihoods and information criteria are relative to one another only on the data which they were evaluated on (which is the cell that is influenced, ergo the likelihoods represent incoming edges). **networkx** calculates the placement of each node, using the connection strength (which can also be negative) to perform a spring simulation, minimizing the difference between intended and actual distance. This placement can be different for each time **plotNetwork** is called. Then, connections are drawn using the **annotate** matplotlib function. Connections that are higher than 90% of the maximum are drawn as solids, higher than 50% are drawn as gray dashed lines and all others as light-gray dotted lines.

The connection matrix that is drawn by **plotConnections** scales dots to show connection strength. Connections from a node onto itself are colored differently (in the example a lighter gray) to make the orientation of the connectivity matrix easily apparent.

4.4.5 statcollector - Collecting Statistics

A **StatCollector** is a data structure that aims to make it easy to collect statistics about models. Essentially it is a dictionary of dictionaries, where the first level indexes the model the statistics is about and the second level the different kinds of values. This seems unintuitive, when one wants to eg. quickly get all likelihoods. But keeping the model in the top level enables one to filter models on certain criterion.

```
import ni
stat = ni.StatCollector()
stat.addNode("Model 0", {'ll_test': -240,
             'll_train': -80,
             'complexity':10})
stat.addNode("Model 0/1", {'ll_test': -100,
              'll_train': -90,
              'complexity':14})
```

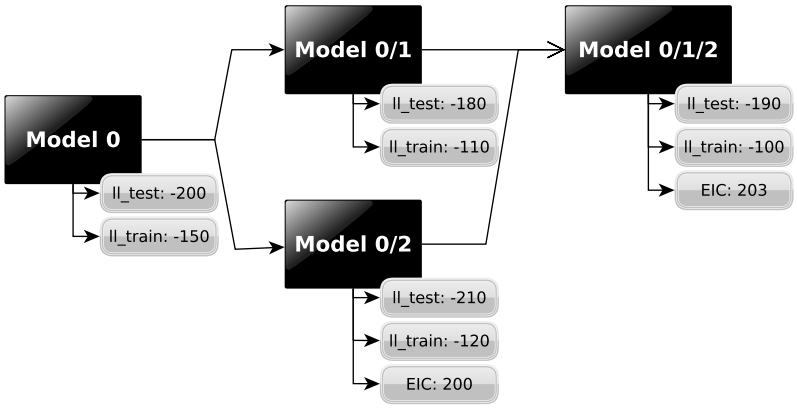


Figure 4.4.8: An example of a StatCollector instance: "Model 0/1" extends "Model 0", which in turn is extended by "Model 0/1/2". Not all models contain all values. In [Konishi and Kitagawa, 2007] on page 87 there is a very similar picture illustrating how adding components to a weather model changes the AIC of the models.

The name of the node identifies the model. Models that extend other models can use a pseudo tree structure by including forward slashes in their name. Values of a specific keyword can be fetched for all models.

StatCollectors allow to filter models either with a prefix string or arbitrary regular expression. Renaming models is also possible with the **rename** method.

Model levels can be pushed into attribute names or attribute prefixes pushed back into model names. Eg. bootstrap evaluations with different data sets will generate the same attributes. To associate them to the same model, the bootstrap function can prefix the names of the attributes with eg. `'dataset1_'`. Alternatively, a new subnode to the model can be created (`'Model 0/1/dataset1'`),

which allows eg. for all test likelihoods to be collected, regardless from which evaluation they come. If the EIC for different datasets is to be compared for one model, one can push the last level of the model name into the attribute name: `'Model 0/1/dataset1'` and `'ll_test'` becomes `'Model 0/1'` and `'dataset1_ll_test'`.

StatCollectors are useful when one wants to plot distributions of values of some evaluation for a range of models that relate to one another.

StatCollectors can be saved and loaded to a file. Also a list of files can be loaded, which are then incorporated into one **StatCollector** instance. Instead of a list a *glob*[6] can be used (a string containing the wild-card character ***** such as `'session3/*.stat'`), which then loads a list of files that match the pattern.

4.4.6 html_view - Collecting and Rendering HTML Output

The hypertext markup language (html) is a very flexible way of setting text and graphics as interactive or non-interactive websites. It builds on an ordered tree structure that holds all elements that are to be displayed. The *jQuery*[7] JavaScript library enables interactive functionalities with few to no lines of code, from simple hiding and showing of elements to animations and complex manipulations of the document tree.

The **View** class offers a simplified tree structure to save output to, which is then rendered as a fully styled html file. The tree structure is instantiated by saving objects to certain *paths*, ie. forward slash separated nodes. If two elements have exactly the same path, the second object overwrites the first one, so some unique identifier should be included in the path. These paths are compiled into an actual tree structure that is parsed by a recursive interpreter, such that arbitrarily nested output can be generated. In this structure, nodes are sorted alphabetically[8] Some node names have special roles and shift the interpreter into a different mode:

tabs
: The keyword `tabs` creates a tabbed interface, such that only one of the children will be displayed at a time. If one tab is selected the focus can be changed with the arrow keys.
Example `'Cells/tabs/1/plot A'`, `'Cells/tabs/2/plot A'` will create two tabs under the title *Cell* labeled with 1 and 2 containing the node `'plot A'` for each cell.

hidden
: The child will be hidden until a link `+ show/hide ...` is clicked.

table
: The children will be displayed in a table, sorted by the next two nodes in the path as rows and columns.

[6] named after an archaic Unix program

[7] see `http://jquery.com/`

[8] with numbers being treated as complete numbers and not digits: $9 < 10 < 100$ instead of $10 < 100 < 9$

#N
: for intergers N changes the order of elements, but is not displayed.
Example: `'Plots/#1/Plot about Zebras'`, `'Plots/#2/Plot about Ants'` will show the Zebra plot before the Ants plot, although normally they would be sorted alphabetically.

Some objects of the **ni.** toolbox contain methods that generate a representation of themselves to be inserted into a **View**. A **FittedModel** eg. will create three tabs, one with the configuration options, one with plots of the design components and one with the fitted design components. A **Data** object will show the mean firing rates across cells and trials and spike plots in a tabbed interface. The default **StatCollector** output is made up out of very broad plots that cover all possible dimensions that are contained in the object. In most cases only a few of those plots are informative.

View is a context manager. If it is initialized with a filepath and used in a **with** statement, the **View** will be rendered to this file, even in case of an exception being raised.

4.4.6.1 Figures in View Objects

Figures can be saved into a **View** via the **.savefig(`path, fig`)** method. It will insert a png image of the plot, encoded in a **base64** string.[9] This makes it possible to have the picture directly embedded in the html file. The image can be saved or copied from any web browser, but no actual image file is created. While this reduces clutter files in the output directory, this can also cause the html file to become as large as a few megabytes and a bit slow to load over a network if a lot of plots are produced, even if they are hidden in tabs.

The **View** class also offers a **.figure(`path`)** method, that returns a context manager, such that a new matplotlib figure is created when the context is entered and this figure is saved in the tree when the context is left.

Like **StatCollector**s, **View** can load lists of files or all files matching a wildcart *glob* pattern.

[9] See `http://en.wikipedia.org/wiki/Base64`

Chapter 5

Bootstrapping an Information Criterion

A problem in statistical modeling is to find a good complexity for a model to predict unseen data most accurately. It is easy to tune a model in such a way that it has a high likelihood on the training set (or even one additional test set, if one tweaks in response to test set evaluation), but this may model not the process in question, but rather the noise in the particular instance of the process.

When additional free parameters are added to a model, the likelihood will become greater - or stay at least equal - since if the new parameter does not explain any previously poorly matched data, it will be just set to 0.

Every model that is obtained by maximum likelihood estimation has a systematic error - a bias - in estimating its own likelihood on training data. This bias needs to be estimated to find out which model is *actually* better. One such method is the Akaike Information Criterion (AIC)[1], another the Bayesian Information Criterion (BIC) and lastly the Extended Information Criterion (EIC).

5.0.7 AIC

The AIC aims to compensate for the bias by taking the number of free parameters into account and adding them as a penalty onto the likelihood. In a set of models, the best model is that which minimizes the AIC estimation:

$$AIC(m, d) = -2l(m, d) + 2k \tag{5.1}$$

Definition from [Akaike, 1973, Akaike, 1974]
m is a model, d is the data and k the number of parameters. $l(m, d)$ is the log-likelihood of the data, given the model.

[1] or An Information Criterion

The AIC is a relative estimate of the information lost when representing a process by a model. It does not give an absolute measure on how good a model is (as would hypothesis testing), but rather a relative comparison. It is derived from the Kullback-Leibler divergence $\left(I(G;F) = E_G\left[\log\left\{\frac{G(X)}{F(X)}\right\}\right]\right)$ as described in [Konishi and Kitagawa, 2007]. Since the true distribution is not known, the KL divergence is simplified to $E_G[\log g(X)] - E_G[\log f(X)]$. Since the measure is only used in relativistic terms, the first term (which is equal for all models that try to approximate g), can be dropped, leaving only the *expected log-likelihood*, which can be approximated with collected data.

In these terms, the best model is the one, which maximizes the log-likelihood on the observed data. But this estimation is heavily biased, as the model will always perform well on the data it was trained on. For every finite set of observed data, the set of parameters $\hat{\theta}$ that is obtained by maximum likelihood estimation, yields an equal or higher likelihood on the observed data than the parameters of the true distribution, even if the process is indeed identical to the model.[Konishi and Kitagawa, 2007, p.54] If one assumes that there exists a θ that makes the model perfectly approximate the process that is to be modeled, it can be shown that this bias approximates the number of free parameters used in the model.

The AIC can be used as a model selection method, just like the maximum likelihood method. Just like the likelihood, AIC changes with the amount of data used to fit the model. In particular, one might notice that when the amount of data used to fit a model is rising, the likelihood drops, as more data means more overall mismatch between data and prediction. But while the likelihood scales in magnitude with the data, the bias is expected to approximate closer and closer to the number of parameters. [Shibata, 1976] claims that with increasing number of observations, even if a more complex model is selected, the coefficients will be closer to their real value - in case of unnecessary coefficients 0.[Konishi and Kitagawa, 2007, p.74]

5.0.8 BIC

The BIC or Schwarz's information criterion, uses posterior probability to select models. This approach is simplified to estimating the *marginal probability*, since all other factors in the posterior probability are equal for all models.

The marginal probability is given by $\int f(x_n|\theta)\pi(\theta)d\theta$, which is approximated as:

$$-2\log\int f(x_n|\theta)\pi_i(\theta)d\theta = -2\log f(x_n|\hat{\theta}) + k\log n \tag{5.2}$$

$\pi_i(\theta)$ is the prior probability of the model with the parameters θ. k the number of parameters, n the number of observations. $f(x_n|\theta)$ is the likelihood of the data, given the model, $f(x_n|\hat{\theta})$ the likelihood given the maximum likelihood estimated model. [Konishi and Kitagawa, 2007, Chapter 9]

The definition of the BIC is very similar to the AIC, but also takes into

account how much data is used for estimating the log-likelihood:

$$BIC(m,d) = -2\log l(m,d) + k\log n \tag{5.3}$$

Where k is the number of free parameters and n the number of observations.

For the amount of observations used in Experiment 1 in 5.1, this will be quite a significant difference to the factor 2 of the AIC.

5.0.9 EIC

The EIC tries to estimate the bias by sampling from the data and extrapolating its features, then fitting the model on both, the original (training) and re-sampled data and estimating how much the training data overestimates its own likelihood. This can be thought of as an exaggeration of the bias, resulting in models that are clearly overfitted to an overrepresented feature in the data.

Using a large number of bootstrap samples $\hat{\mathbf{d}}$, obtained by the bootstrap transformation $\mathbf{T}$, each giving rise to a fitted model $\hat{\mathbf{m}}$, the EIC criterion is calculated by estimating the expected bias as a mean of all bootstrap biases $l(\hat{\mathbf{m}},\hat{\mathbf{d}}) - l(m,\hat{\mathbf{d}})$ to the model m fitted on the actual data d.

$$EIC_T(m,d) = -2l(m,d) + 2[l(\hat{\mathbf{m}},\hat{\mathbf{d}}) - l(m,\hat{\mathbf{d}})] \Big| \begin{array}{l} \hat{\mathbf{d}} = T(d) \\ \hat{\mathbf{m}} = fit(\hat{\mathbf{d}}) \end{array} \tag{5.4}$$

m is a model, d is the data, $\hat{\mathbf{m}}$ a model fitted on one particular bootstrap sample $\hat{\mathbf{d}}$, which was obtained by using T on d. $l(m,d)$ is the log-likelihood of the data, given the model. T is a bootstrap transformation.

Note that the Data has to be of the same size for d and $\hat{\mathbf{d}}$.

A bootstrap transformation can be a simple jack knife operation that takes one of the samples out or a a trial based reshuffling of the data. Also one can re-sample the data from a previously made model.

In [Konishi and Kitagawa, 2007, Chapter 8.3] a *Variance Reduction Method* is discussed that was introduced in [KONISHI and KITAGAWA, 1996]. The extended formula 5.5 (equivalent to [Konishi and Kitagawa, 2007, p.199], equation 8.28) takes into account the difference of the bootstrap model $\hat{\mathbf{m}}$ and the actual model m on both, the bootstrap data $\hat{\mathbf{d}}$ and the actual data d. This can result in a faster convergence than only the evaluation on the bootstrap data.

$$EIC_T(m,d) = -2l(m,d) + 2\left[l(\hat{\mathbf{m}},\hat{\mathbf{d}}) - l(m,\hat{\mathbf{d}}) - [l(\hat{\mathbf{m}},d) - l(m,d)]\right] \Big| \begin{array}{l} \hat{\mathbf{d}} = T(d) \\ \hat{\mathbf{m}} = fit(\hat{\mathbf{d}}) \end{array} \tag{5.5}$$

$l(\hat{\mathbf{m}}, \hat{\mathbf{d}})$ and $l(m, \hat{\mathbf{d}})$ are the log-likelihood of the bootstrap-sample fitted model and the actual data fitted model on the bootstrap sample.
$l(\hat{\mathbf{m}}, d)$ and $l(m, d)$ show the log likelihood of the actual data, given the bootstrap sample/actual data fitted model.

However, there can be a large asymmetry between the bias $l(\hat{\mathbf{m}}, \hat{\mathbf{d}}) - l(m, \hat{\mathbf{d}})$ on the bootstrap data and $l(\hat{\mathbf{m}}, d) - l(m, d)$ on the normal data, depending on the transformation.

As a bootstrap transformation, one can reshuffle trials instead of time points, which will result in less data that is very similar to the original data. In the following sections, specifically Section 5.1.1.7, the implications of this change are discussed. Also one can approximate the distribution of spike trains of which we want to sample more data by a model of varying complexity. This leads to not a single EIC, but to a range of different criteria that differ in their function and feasibility (Section 5.0.9.2 will extend on this notion).

The EIC is also used by the R-package *reams*[2], which uses a resampling of observations, for model selection. It uses the *leaps* exhaustive search regression fit.

5.0.9.1 Resampling by Creating More Spike Trains

Instead of sampling from instances of time points or complete spike trains, it is also possible to sample from the probability space of the process that is under investigation. This requires a model of the process, from which new spike trains can be generated. This will however also give different results than physically sampling from the actual process, since the model and the process will diverge in some aspects. But from this, even more can be inferred about the model, as the fact that some models have an asymmetric bias compared to the generated data and others might not, gives insight into whether a model is able to pick up statistics that are (by their generative process) really present in the data.

5.0.9.2 A Range of Criteria

The EIC can be used with a variety of bootstrap transformations and as one of two equations. The Equation 5.4 provides the conservative estimation, while 5.5 will reduce the variance and converge faster, but introduce a second source of variability, which in theory should balance the first, but might behave differently.

As a transformation it is possible to use one of the following methods, resulting in two EIC criteria each:

- Resampling based on the original data
  - redrawing time points
    - → conservative EIC using time reshuffle (EIC)
    - → variance reduced EIC using time reshuffle ($vrEIC$)

[2] http://cran.r-project.org/web/packages/reams/index.html

- redrawing trials
  - → conservative EIC using trial reshuffle (EIC_{trials})
  - → variance reduced EIC using trial reshuffle ($vrEIC_{trials}$)

- Model based resampling
  - using simple models
    - → conservative EIC using a simple model (EIC_{simple})
    - → variance reduced EIC using a simple model ($vrEIC_{simple}$)
  - using complex models
    - → conservative EIC using a complex model ($EIC_{complex}$)
    - → variance reduced EIC using a complex model ($vrEIC_{complex}$)

This gives rise to 8 kinds of EICs. The model based resampling has a clear disadvantage in that it needs a fitted model, which extends the computational requirements by another task. However, it might be that only those models can provide adequate approximation to the data, such that the EIC produces meaningful values.

To investigate this, experiments were conducted, calculating each of the EIC for different bootstrap transformations and comparing the results.

The following table 5.1 gives another overview about the used EIC values:

	conservative EIC (Eq. 5.4)	variance reduced EIC (Eq. 5.5)
time based reshuffling	EIC	$vrEIC$
trial based reshuffling	EIC_{trials}	$vrEIC_{trials}$
simple Model	EIC_{simple}	$vrEIC_{simple}$
complex Model	$EIC_{complex}$	$vrEIC_{complex}$

Table 5.1: Different variants of the EIC. The EIC without subscript is the original definition, while $vrEIC$ incorporates the variance reduction method of [KONISHI and KITAGAWA, 1996]. The variants with subscript describe alternative bootstrap transformations.

5.1 Experiment 1

The bias in the likelihood estimation of likelihood maximized models is systematically higher than the actual likelihood. However it might vary from model to model and different data statistics. A different model might have a different bias due to complexity and the nature of the components that make up the model. Also a model might have a different bias on data with different statistics as certain regularities in the data might be easier or harder to pick up by the model. Also the amount of noise that *looks* like an important property of the data plays a role, as well as the tendency of the noise to cancel out.

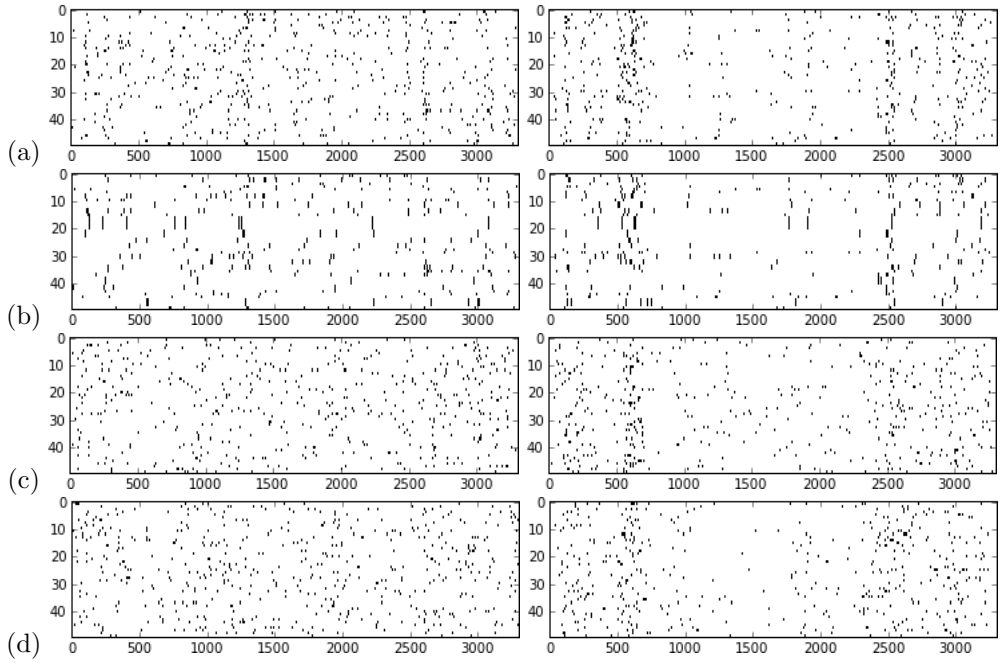


Figure 5.1.1: Sets of 50 trials for cell 0 and cell 5: (a) original data (b) Trial shuffled data, (c) generated with a simple autohistory model and (d) generated with a complex crosshistory model

Since the kind of bootstrap transformation may lead to different results, five different kinds of bootstrap data $\hat{\mathbf{d}}$ were used (see also 5.1.1). One additional bootstrap method to the four mentioned in table 5.1 was used, as by an implementation error the time reshuffle was only performed on the independent, yet not on the dependent variable. This additional bootstrap data will not contain the statistical relationship between independent and dependent variables that the model is supposed to pick up and can act as a control for how important mimicking the original data actually is.

The experiment uses the following 10 versions of EIC:

- time shuffled data (EIC and $vrEIC$)
- trial shuffled data (EIC_{trials} and $vrEIC_{trials}$)
- data, in which the relationship between independent and dependent variable is destroyed (conservative EIC using unrelated data ($EIC_{unrelated}$) and variance reduced EIC using unrelated data ($vrEIC_{unrelated}$))
- data generated by a simple model (EIC_{simple} and $vrEIC_{simple}$)
- data generated by a complex model ($EIC_{complex}$ and $vrEIC_{complex}$)

Of each kind of bootstrap data 50 sets of 50 trials of newly generated data were created. Two multi channel models were fitted on the dataset, one using rate and autohistory and one additionally using higher order autohistory and full crosshistory components. Each of these models then generated 50×50 trials, which were saved into files.

Trial and time shuffling was done on-the-fly, without generating and saving data to the network storage, which has the effect that the trials will have a different order for all evaluations. In contrast the generated data will have the same order of trials for all evaluations.

Then models were created, modeling one out of the 11 neurons, once only with their own autohistory, then with each of the other cells, then with each ordered pair of other cells, yielding 737 models[3]. Each model was **bootstrap** evaluated with $\hat{\mathbf{d}}$, half of the data as training and half as test data.

The experiments were run on the IKW grid with a maximum of 100 jobs submitted at a time. The fitting of the bootstrap models was done in one job per cell to fit, as these computations are independent. The generation of 50 trials each was also done in parallel. Bootstrapping was done as one job for each model, as the evaluation has to fit the model on original data first to compare it to the bootstrap fitted models. To only fit the model on the original data once, it was necessary to run each evaluation as one job.

The resulting information criteria were used to infer connections by calculating the information gain from the simple model to a model containing a certain cross-component. This gain was then thresholded with 90% of the maximal gain to show differences in how the information criteria evaluate each interaction.

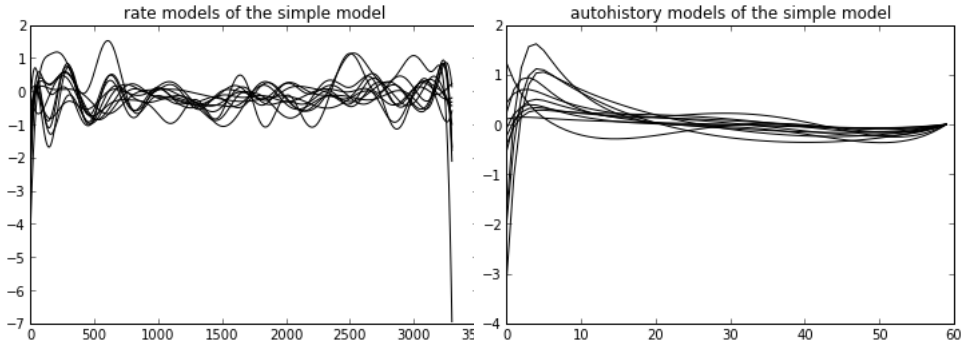
The source code for this experiment can be found in the toolbox as an example project.

5.1.1 Results

5.1.1.1 Fitted Multi-Model

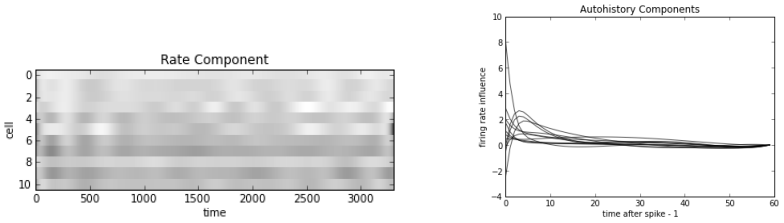
The model that generated the simple data is visualized in 5.1.2 and the one for the complex data in 5.1.3.

[3] 11 autohistory models $+11 \times 10$ with one crosshistory component $+11 \times (11 + \frac{10*9}{2})$ with two history components

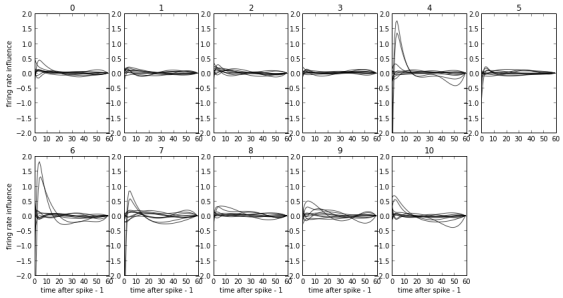


(a) Rate Components (b) Autohistory components

Figure 5.1.2: Components of the created simple model: (a) the rate components (b) the autohistory components



(a) Rate Components (b) Autohistory components



(c) Crosshistory components (same scale across all plots)

Figure 5.1.3: Components of the created complex model: (a) the rate components show some fluctuations that are equal for the different cell assemblies. Some assemblies seem to have a lower firing rate overall. (b) in the autohistory components there is generally a positive interaction, similar to the exponential decay in the interspike interval histogram of the data. Some assemblies show an initial inhibition. (c) shows that some cells are strongly driven by other cells. There seems to be little negative correlation. The 2d autohistory is not shown.

5.1.1.2 Information Criteria

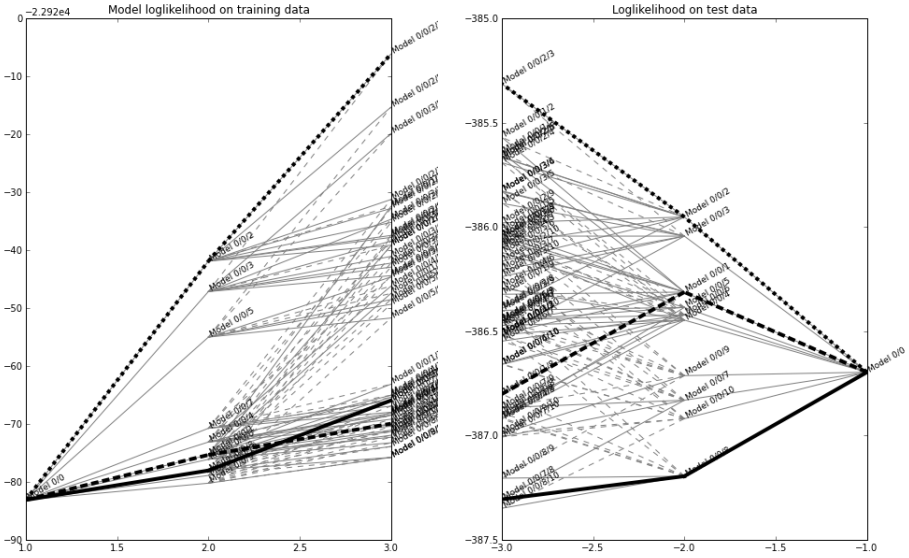
How the different criteria evaluate models relative to one another can be seen best in tree plots[4], which take the simpler models as roots from which the more complex models evolve - either from left to right or from right to left. The vertical axis represents one of the information criteria, such that if a model improves on its predecessor, it will be higher up, if it is worse, it will be lower.

The lines connecting the models are either solid or dashed, depending on which model they come from, such that in the third level each model receives two lines: one dashed, one solid.

On the next few pages a few of those figures are drawn which are afterwards discussed.

To make comparison a bit easier, some plots are plotted from left to right, others from right to left in complexity, such that two comparable trees can be seen as mirror images.

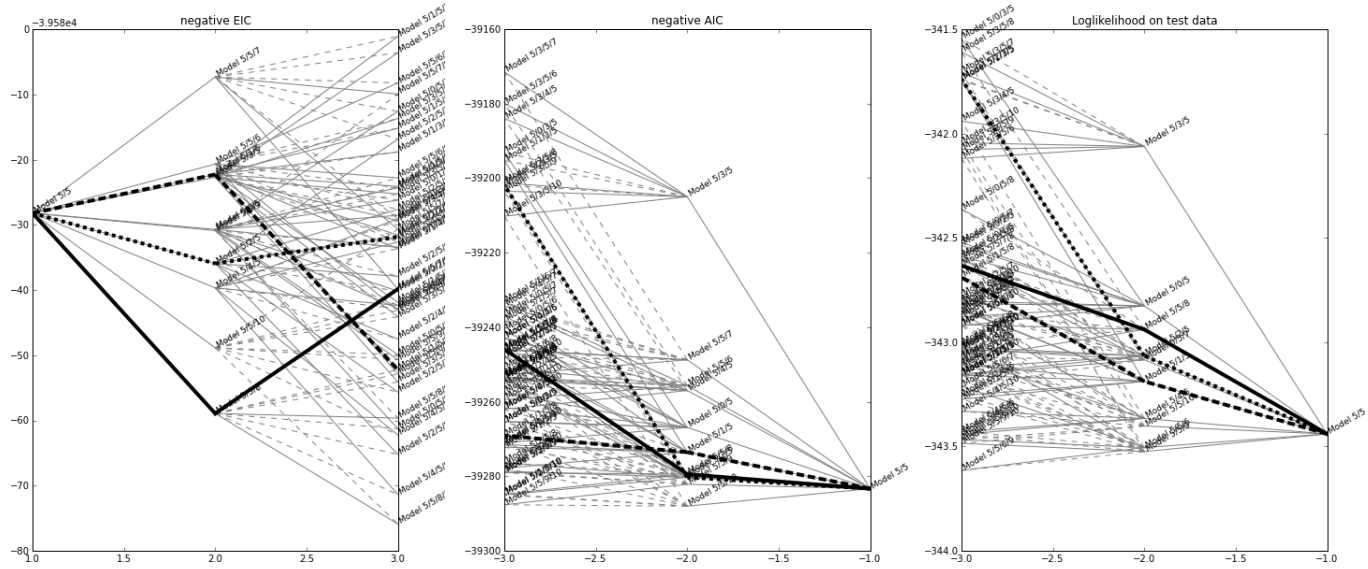
[4] actually they more or less resemble the structure of a partially ordered set/lattice



(a) Likelihood on the training data is steadily increasing

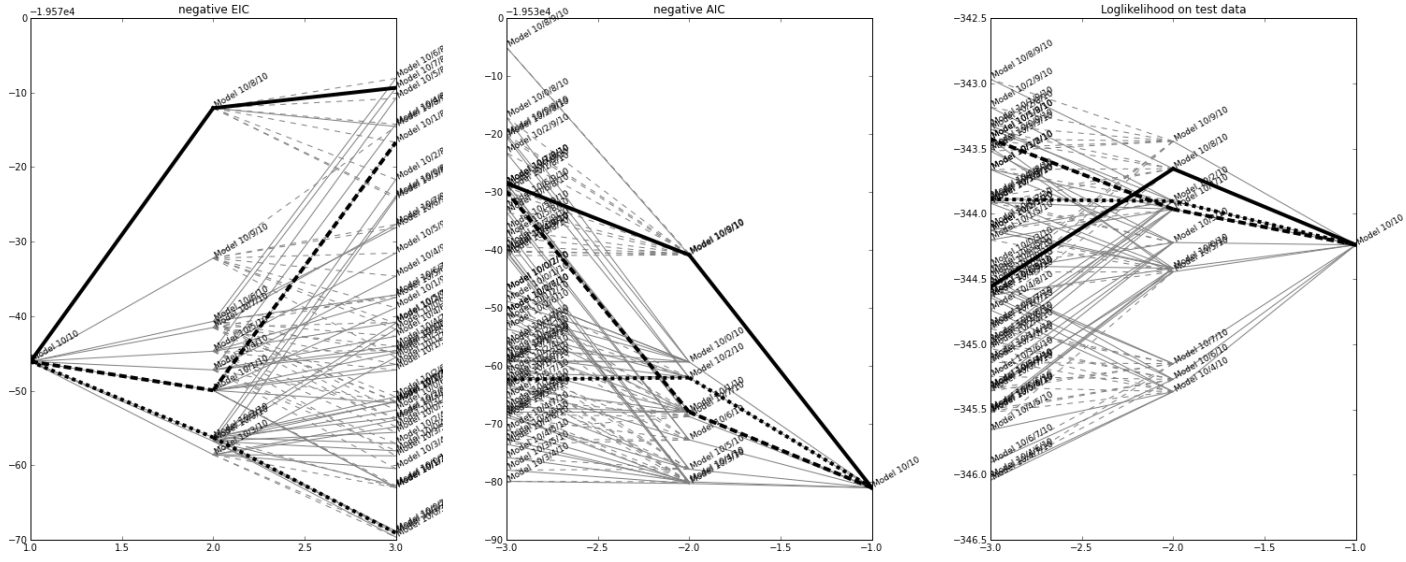
(b) Likelihood on the test data sometimes increases, but also decreases

Figure 5.1.4: The likelihood behaves differently for unseen data, than for the data the model was trained on. The plots highlight three models, rising in complexity. The dotted line is rising confidently for the training data, and for the test data, each added component also increases likelihood. The dashed line also rises strictly monotone for the training data, however on the test data the first component provides an increase, while the second results in a decrease in test data likelihood, which brings it below the level of likelihood of the initial model without both components. The solid line is rising higher than the dashed line in the training data, but on the test data it performs worse and worse with both components added.



(a) negative $vrEIC_{complex}$ (b) negative AIC (c) test loglikelihood

Figure 5.1.5: comparing an EIC ($vrEIC_{complex}$), AIC and test likelihood for Models on cell 5. See Section 5.1.1.3 and following for a discussion.



(a) negative $vrEIC_{complex}$ (b) negative AIC (c) test loglikelihood

Figure 5.1.6: comparing an EIC ($vrEIC_{complex}$), AIC and test likelihood for Models on cell 10. See Section 5.1.1.3 and following for a discussion.

5.1.1.3 A First Look at the Information Criteria

Since the EIC was bootstrapped, it is interesting to know, how much variance is to be expected after a certain number of bootstrap samples are drawn. Figure 5.1.7 shows for two cells how the EIC (for the complex generated data) for all models changes less and less with each new bootstrap sample. Comparing the changes per sample with the scale of the values in the examples, the changes becomes negligible for the comparison of most of the models. Also the models tend to move together for the most part, so even a large change for one model might also affect all other models to move in the same direction.

Inspecting a tree view of the models, one can easily see, that with increasing complexity, the likelihood on the training data increases as well (see Figure 5.1.4a). This is plausible, as adding new components can not make the model perform worse if the likelihood is maximized. It would be ignored, if it added no new explanatory value, but as it most likely will increase the fit in some way, the likelihood is steadily rising.

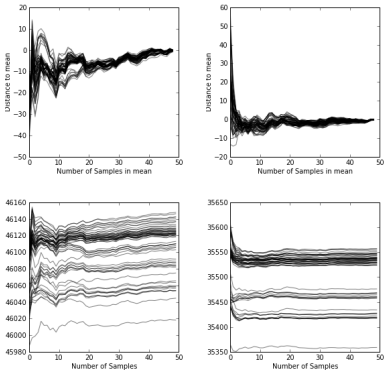


Figure 5.1.7: Two examples of how the mean EIC converges (here $vrEIC_{complex}$): The changes of the mean with every new bootstrap trial get smaller and smaller.

However, if we consider the likelihood of the models on previously unseen data, we get a different picture. Some models perform better than their less complex predecessors, but just as many perform worse (see Figure 5.1.4b). This is caused by the models modeling not an essential part of the data, but a non-informative noise part. The models are *over-fitting*. The apparent *good* fit on the training set is only due to the bias of likelihood estimation with maximum likelihood estimated models.

If one takes the likelihood on the test data as an unbiased "ground truth", the information measures EIC and AIC can be compared in how they compensate the bias on the training data. Figures 5.1.5 and 5.1.6 show how different models perform on the test data and in each information criteria. EIC and AIC are shown as negatives, such that a higher value signifies a better model.

5.1.1.4 AIC

It is notable that AIC seldom compensates strongly enough that the least complex model (using only rate and autohistory) can compete with the more complex models. However the simple model seems to be close to the mean performance for cells 0,3,9 and 10, while 2,4,6,7 having it near the mean of the poor performing models. Only on cells 1,5 and 8 the simplest model is among the worst models performing on the test data. The AIC however consistently

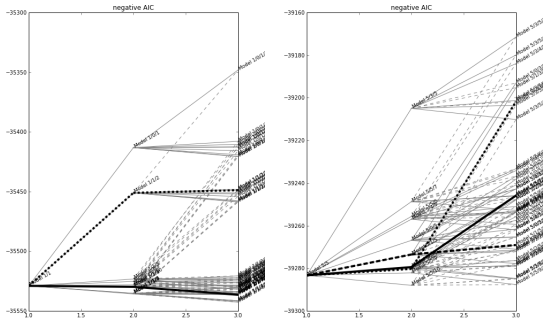


Figure 5.1.8: negative AIC of the models for cell 1 and 5

underestimates the simpler models.

5.1.1.5 BIC

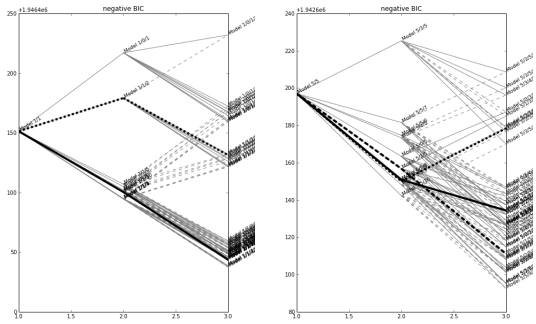


Figure 5.1.9: negative BIC of the models for cell 1 and 5

The BIC compensates very strongly for complexity. The simplest model is in the upper half of models almost always. For cell 3 and 10, it even is the best chosen model. Figure 5.1.9 shows two examples of how strongly the BIC *tilts* the training likelihood plot compared to Figure 5.1.8. The increase in likelihood for the cell 5 model 5/3/5 to 5/3/5/7, which is a big improvement for the AIC, is judged to not outweigh the increase in complexity by the BIC.

5.1.1.6 EIC

The EIC tends to compensate well for the complexity and often[5] has an almost equal split of more complex models enhancing and worsening the simpler model. Spreading out in the hierarchy, one notices that if two models are evaluated as quite good, their "offspring" model (incorporating all components of the previous models) has an even better EIC. It seems that the information gain from the simple model to the first crosshistory component can be translated roughly to that from the first to the second crosshistory component, which, however, is a property that seems to carry from the likelihood on the training data, rather than the bias correction.

In the following, we have to differentiate the different distributions that were used for drawing bootstrap samples.

5.1.1.7 $vrEIC$ - Trial Reshuffling vs. Time Reshuffling

The trial shuffled $vrEIC_{trials}$ compensated for complexity, but not as strongly as the BIC. For most cells, it signifies only one to two interactions as improving on the simple model. For cell 2, 5, 8 and 9, the best model has only one crosshistory component. Those would hint at a causal interaction $0 \rightarrow 2$, $3 \rightarrow 5$, $10 \rightarrow 8$, $10 \rightarrow 9$.

Cells 1, 3, 4, 6 and 7 give the best EIC value to a double crosshistory, while 0 and 10 rate the simple model as worse than at least three crosshistory models.

An example of a graph that might be inferred by model selection of the EIC with trial reshuffling can be seen in Figure 5.1.10

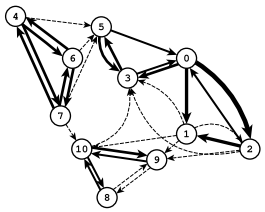
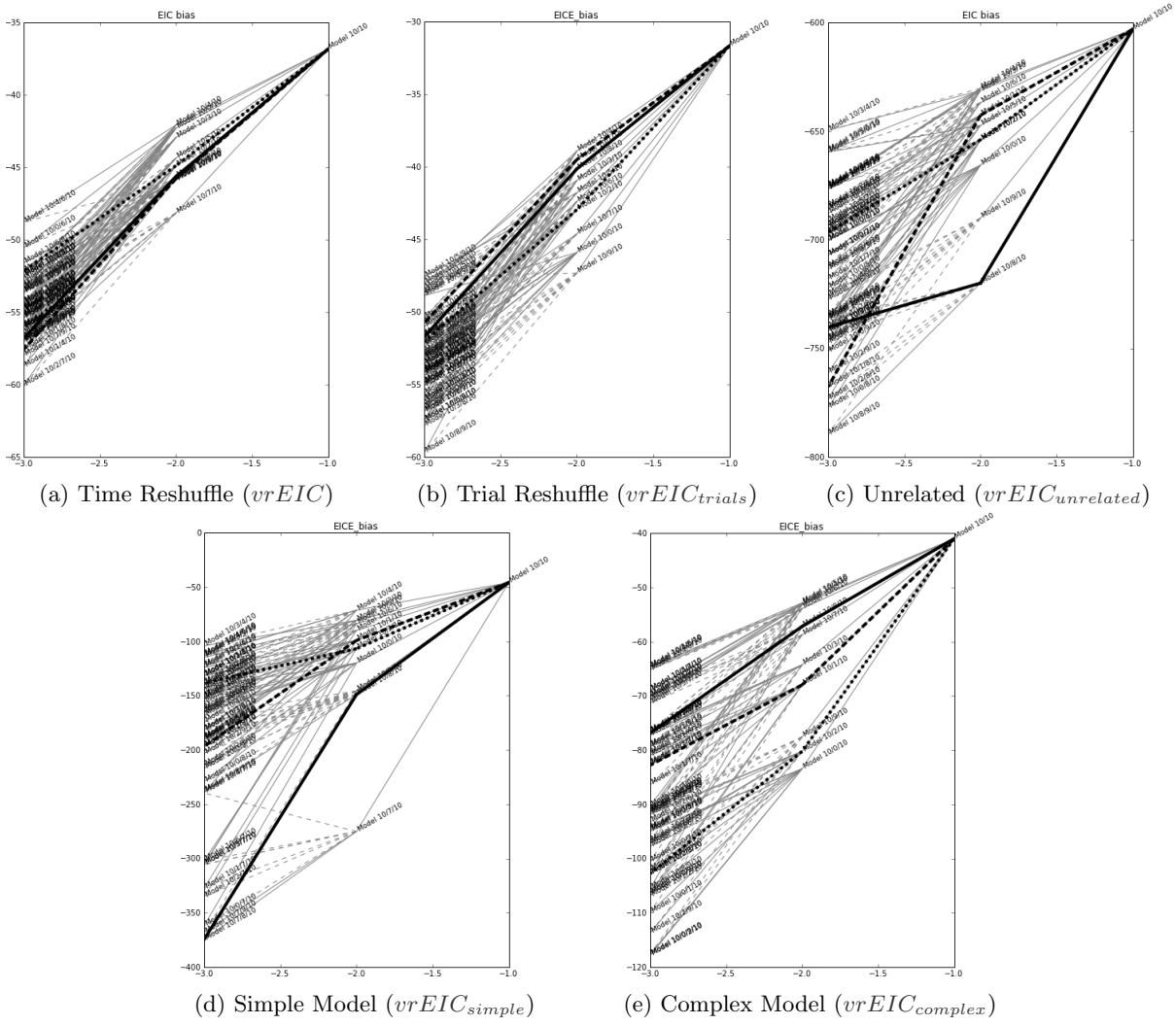


Figure 5.1.10: an inferred graph from EIC with trial shuffling

[5] when exactly will be discussed shortly



(a) Time Reshuffle ($vrEIC$) (b) Trial Reshuffle ($vrEIC_{trials}$) (c) Unrelated ($vrEIC_{unrelated}$)

(d) Simple Model ($vrEIC_{simple}$) (e) Complex Model ($vrEIC_{complex}$)

Figure 5.1.11: The variance reduced EIC **biases** (and only the biases) for cell 10. While the AIC bias would be just a straight line, the EIC calculates the bias on the basis of the bootstrap distribution, which is why the scale is very different for all shown examples: The maximal bias correction for (a) is -60, for (b) it's about the same, for (c) -800, for (d) it's -400 and for (e) -120. The lowest bias (in all cases the simplest model) is for (a) -37, (b) -33, (c) about -600, (d) -52 and for (d) -40. Not only do the ranges of bias correction differ, the actual models that get a higher or lower correction is also different for each EIC version. For the simple and complex model EIC, this means that more complex models can actually receive a *lower* bias correction than a particularly bad less complex model, in some cases even if the more complex one is an extension of the simpler model (see the dashed line going back up from Model 10/7/10 in (d)).

5.1.1.8 $vrEIC_{simple}$ - The Simple Model

The simple model generated data produces the best $vrEIC_{simple}$ for the simple model. This is no surprise, as this model essentially created the data, so additional parameters can hardly add any explanatory value.

Some models trained on cell 4, 6 and 7 are judged as almost as good as the simple model. But Model 4/4/6 (having 4 as autohistory and cell 6 as a crosshistory component), while being highly praised by evaluation on the test data, is considered a bad model by the $vrEIC_{simple}$. The Model 6/4/6 on cell 6 also has a very high likelihood on the test data, but is regarded by the $vrEIC_{simple}$ as pretty bad.

The simple model did not model any crosshistory, so any relation between the spikes in 4 and 6 in the bootstrap data can only be a correlation due to firing rate (eg. mutual fluctuations). However in the real data, there might be an actual causal relation. This leads the variance reduction term of the $vrEIC_{simple}$ to penalize this model with a large bias, as the real model is far better at predicting the actual data and the term $-[l(\hat{\mathbf{m}}, d) - l(m, d)]$ will be very large (ie. positive, adding to the penalty).

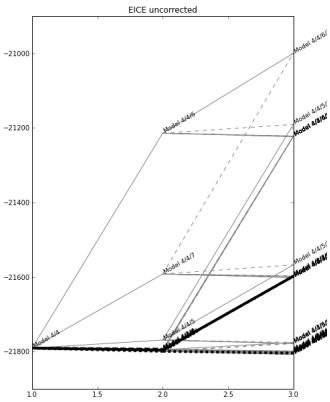


Figure 5.1.12: conservative EIC_{simple}

If the EIC would have been calculated by Equation 5.4, the models 4/4/6 and 6/4/6 would far outperform the simpler model (as seen in the conservative EIC_{simple} plot 5.1.12).

But since the $vrEIC_{simple}$ reduces variance using both directions, the divergence between bootstrap data and real data results in a very large bias being calculated for these actually good models on the basis of using the simple model as a bootstrap mechanism.

This divergence between the test data likelihood and EIC estimates also hints at the fact that important structure in the data is lost, if the sampling process ignores all cross-causalities. This however is not an insight about the models being tested, but about the bootstrap data and the model that generated it.

5.1.1.9 $vrEIC_{complex}$ - The Complex Model

The $vrEIC_{complex}$ computed with the complex model seems to split the models relative equally in good and bad additions to the model. Some components improve the $vrEIC_{complex}$ value significantly. A good component added to a good model will give an even better model, while components that tend to overfit reduce the $vrEIC_{complex}$ value.

5.1.1.10 The EIC Bias

Figure 5.1.11 shows how the different EIC biases are distributed. With rising complexity, the bias that is corrected also increases. However in contrast to the

AIC, the bias of each model depends heavily on the statistics on which it was evaluated.

The trial reshuffled $vrEIC_{trials}$ gives a distribution such that the increase in bias from the simple model is spread in a range from 7 to 17. The spread is roughly maintained one complexity level further. But some models even The $vrEIC_{complex}$ computed on the complex model has a wider spread, and keeps spreading further, while some models get a smaller bias with the inclusion of an additional component.

5.1.1.11 Information Gain and Network Inferences

The different information measures give different weight to the simple model. This gives insight in whether the criterion thinks that a certain interaction component can improve the model or whether it will lead to over fitting. If the more complex model has a better value than the simple model, there is an information gain in including this component in the model.

The gain can be thought of as a split in the tree plots along a line going through the simple model horizontally.

Gain of:	≤ 0	> 0	percentage split
Training likelihood	0	110	0 / 100%
Test likelihood	47	63	43 / 57%
AIC	37	73	34 / 66%
BIC	95	15	86 / 14%
conservative EIC reshuffle trials	58	52	53 / 47%
conservative EIC reshuffle time	67	43	60 / 40%
conservative EIC reshuffle unrelated	43	67	39 / 61%
conservative EIC simple model	37	73	34 / 66%
conservative EIC complex model	44	66	40 / 60%
variance reduced EIC reshuffle trials	38	72	35 / 65%
variance reduced EIC reshuffle time	52	58	47 / 53%
variance reduced EIC reshuffle unrelated	104	6	95 / 5%
variance reduced EIC simple model	110	0	100 / 0%
variance reduced EIC complex model	65	45	59 / 41%

Table 5.2: Number of connections with a non-positive and positive gain for the different information criteria. A gain smaller than 0 means that the information criterion prefers the simpler model to the more complex model. The *conservative EIC* is calculated by Equation 5.4, while the *variance reduced* $vrEIC$ is calculated by Equation 5.5

Figures 5.1.13a and 5.1.13b show a thresholded network inference from only the likelihood of the test data and training data. The graph using the (unbiased) likelihood on the test data should act as a guideline when interpreting the other graphs. The graph of the likelihood on the training data assumes a larger gain (since it is biased towards more complex models), which means that all connections are included. Because of the scaling only the highest connections are plotted as black solid lines to make them comparable to the other

plots. The training likelihood, after setting a threshold, detects four networks: $\{0, 1, 2\}, \{3, 5\}, \{4, 6, 7\}$ and $\{8, 9, 10\}$.

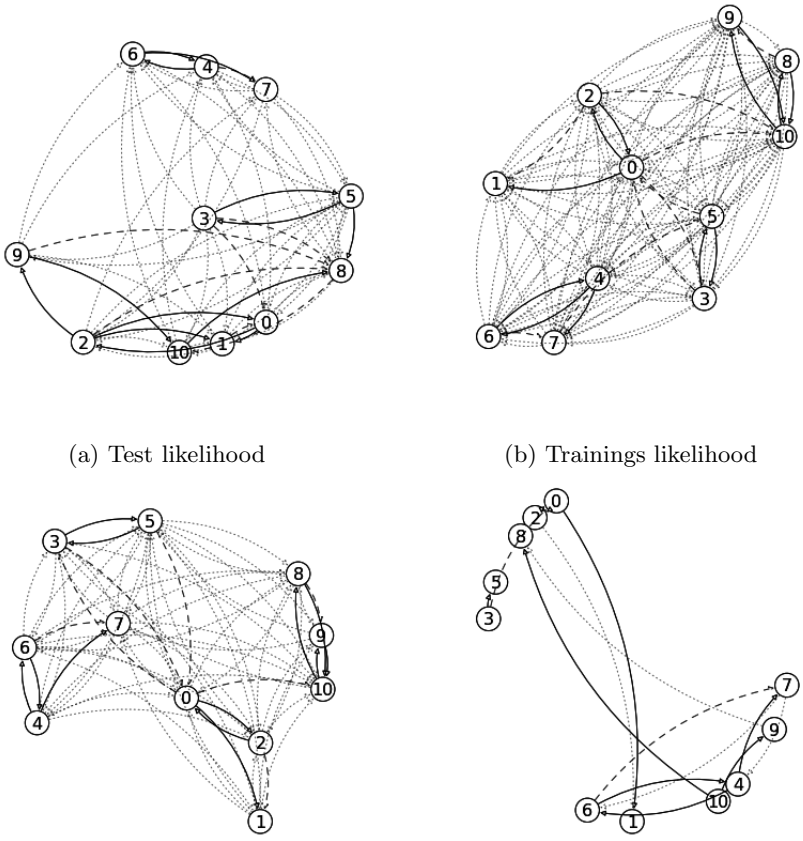
In the likelihood estimation with unseen test data, the groups $\{0, 1, 2\}, \{3, 5\}$ and $\{4, 6, 7\}$ are also found, the group $\{8, 9, 10\}$ however is deemed to be less connected. Some new connections are inserted as also very beneficial, connecting cell 2 to 1 and to 9 and 5 to 8.

The AIC finds the same networks as the training likelihood. This is because the AIC is only bias correcting for complexity, which does not change the order of the models. Some of the models that had a low gain in the graph 5.1.13b are now excluded as their gain in likelihood is less than the AIC bias of adding a crosshistory component.

The BIC selects only a few connections as having a positive gain (Figure 5.1.13d). From the grouping of the nodes it becomes apparent that some of the connections have a quite large negative gain, separating the nodes into two assemblies, which are in itself not well connected.

The trail reshuffling $vrEIC_{trials}$ finds essentially the same subnetworks as the trainings likelihood, however the threshold is lowered a bit as the significant models are grouped closer together.

Figure 5.1.14d shows how the $vrEIC_{simple}$ depending on the simple model disregards all connections as not providing any additional information.



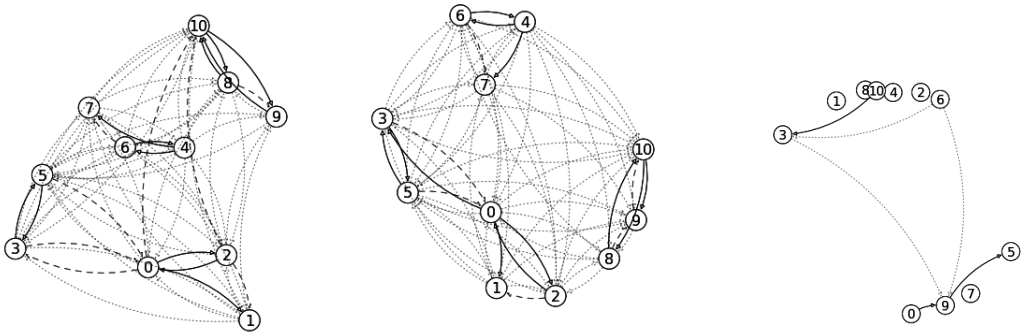
(a) Test likelihood

(b) Trainings likelihood

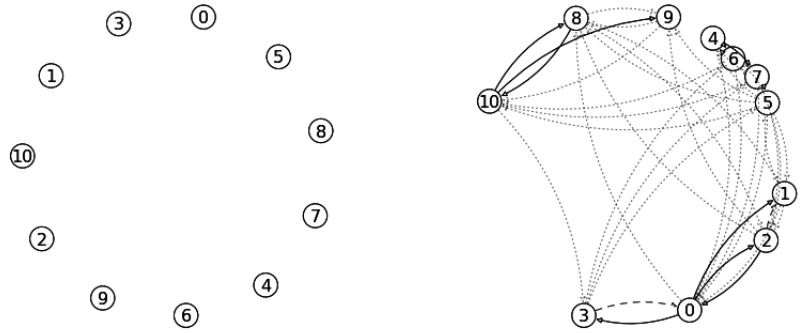
(c) **AIC**

(d) **BIC**

Figure 5.1.13: Networks inferred by different information criteria. The number of connections can be seen in Table 5.2. It ranges from full connection (even if only a few are drawn bold) in 5.1.13b to no connections for 5.1.14d.

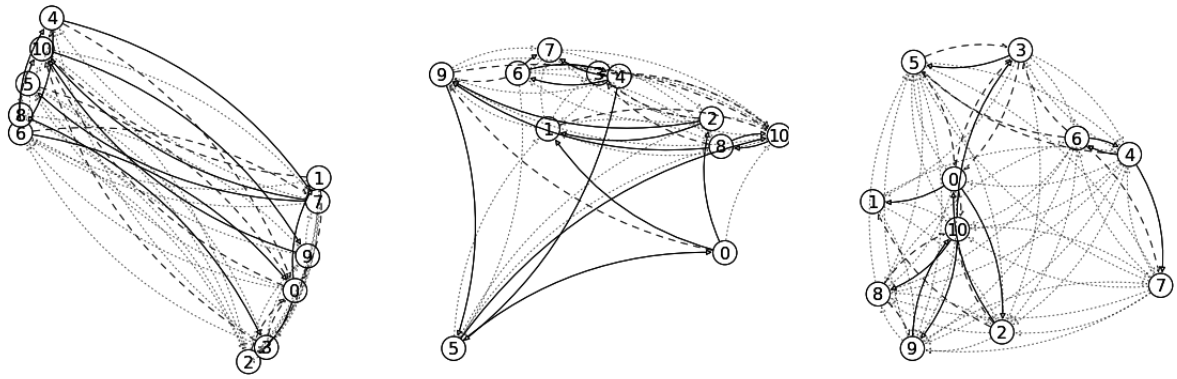


(a) $vrEIC$ sampling **timepoints** from the data (b) $vrEIC_{trials}$ sampling **trials** from the original data (c) $vrEIC_{unrelated}$ sampling unrelated to the data



(d) $vrEIC_{simple}$ sampling from the **simple** model (e) $vrEIC_{complex}$ sampling from the **complex** model

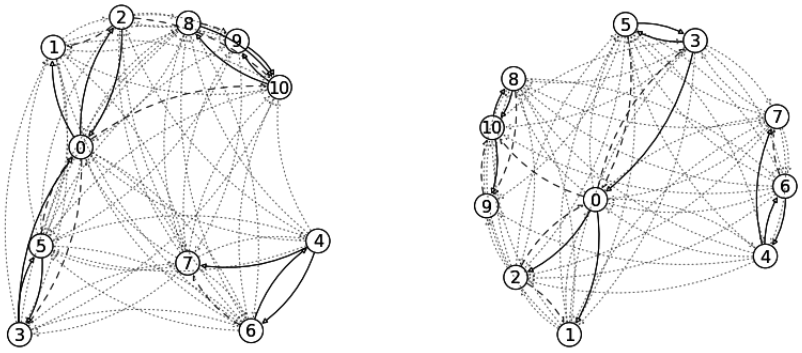
Figure 5.1.14: Networks inferred by different information criteria. The number of connections can be seen in Table 5.2. It ranges from full connection (even if only a few are drawn bold) in 5.1.13b to no connections for 5.1.14d.



(a) EIC sampling **timepoints** from the data

(b) EIC_{trials} sampling **trials** from the original data

(c) $EIC_{unrelated}$ sampling unrelated to the data



(d) EIC_{simple} sampling from the **simple** model

(e) $vrEIC_{complex}$ sampling from the **complex** model

Figure 5.1.15: Networks inferred by the simple version of the EIC. The trial shuffled EIC looses connections (compare to 5.1.14b). All other versions of the EIC gain more connections. This evaluation however might not be saturated, as the simple version of the EIC needs longer to converge.

5.1.2 Discussion

AIC tries to compensate only for complexity as the length of the coefficients vector. If this could be used reliably for model selection (even with arbitrary weights of how much complexity should be weighted), models of one complexity class would remain in their order after bias correction. However, different models have different biases on different data, as shown by simple cross evaluation.

When using the bias corrected likelihood on the training data as a network inference technique, the differences in the order of models is very small. Only the decision which connections to include at all can be assisted with with the different information criteria.

There is a very large difference in the behavior of the trial-shuffled and the time-shuffled $vrEIC$ and the unrelated shuffling $vrEIC_{unrelated}$. This can be expected to some extend, as the unrelated shuffle destroys the statistical properties of the data, while the trial or time point shuffle preserves it. In fact for the connectivity plots, $vrEIC_{unrelated}$ behaves very similar to the simple model $vrEIC_{simple}$. Both take the simple model to be most robust and hence discard assumptions connectivity.

Yet, the $EIC_{unrelated}$ *does* show connectivity, as does EIC_{simple}. Although there was no statistics in the bootstrap data, that would hint at the connectivity, Equation 5.4 seems to be robust enough to still provide meaningful values. In Section 6.2 this will be discussed further.

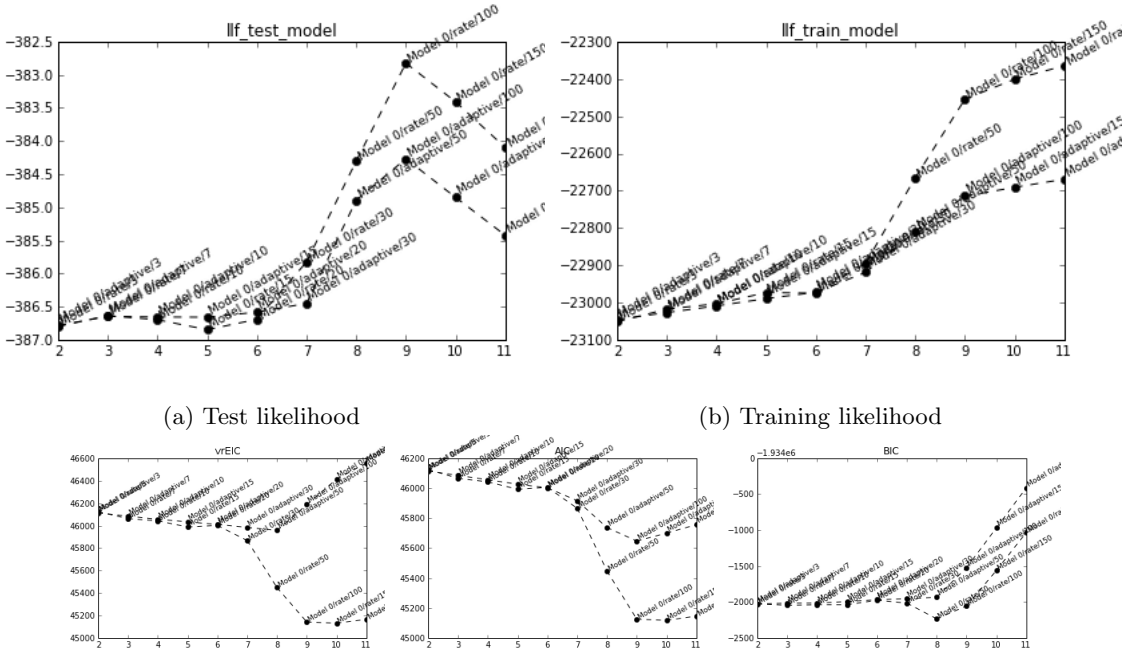
5.2 Experiment 2 - Using Information Criteria for Parameter Selection

To give another application to information criteria, consider the common case of answering the question how many basis splines should be used to model the rate fluctuations in a certain set of data. Normally, one would use a simple cross evaluation for this. However, if data is precious (eg. if some further model selection process requires fresh data as bootstrapping is not possible), one has to resort to using transformed versions of the training data and compensate for the bias as good as one can.

The source code for this experiment can be found in the toolbox as an example project.

5.2.1 Results

The models up to 100 knots get continually better. This can be seen in the test data likelihood plot in Figure 5.2.1a. It may be interesting that the linearly spaced rate component seems to fit the data better than the adaptive rate, which might hint at an error in the implementation, or it might be the case that for this set of data, the resolution should not be scaled with the firing rate. But for the comparison of information criteria even a defective adaptive rate component can be useful, as we know the likelihood of those models on test data.



(a) Test likelihood

(b) Training likelihood

(c) $vrEIC_{trials}$

(d) AIC

(e) BIC

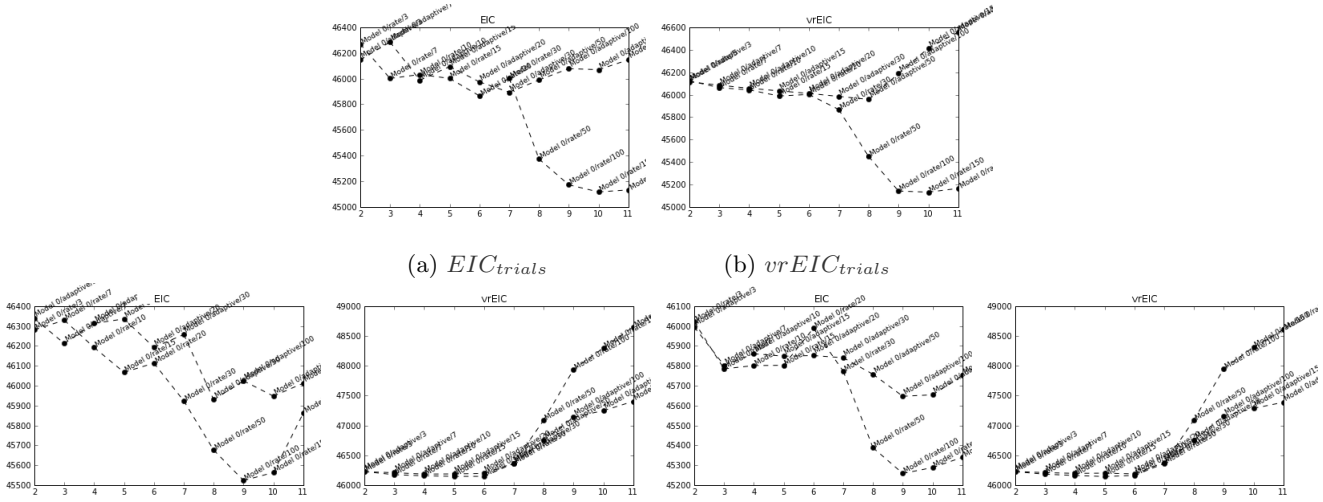
Figure 5.2.1: This experiment shows how the information criteria can be used to find an optimal parameter such as the number of knots of a rate component. The training likelihood rises continually while the test likelihood falls again after 100 knots. The goal is to find an information criterion that will identify the bias such that the maximum in test likelihood coincides with an optimum in the information criterion.

The BIC has a global minimum for the lin-spaced rate at 50 knots, with 100 knots being evaluated as second best. For the adaptive rate, there is a plateau for the small knot numbers and a worsening after 50 knots.

The AIC finds a minimum for the adaptive rate at 100 knots, for the lin-spaced rate a plateau after 100 knots implies an equal weight off between likelihood gained and complexity.

For the EIC values, one has to differentiate again. $vrEIC_{trials}$ shows a strong divergence between adaptive and lin-spaced rate models. The adaptive models are judged similar to the BIC, the lin-spaced models similar to the AIC.

The EIC_{trials} and $EIC_{complex}$ show a large amount of variance, such that local minima can not really be interpreted. $EIC_{complex}$ has a large global minimum for the lin-spaced rate models around 100 knots. $vrEIC_{complex}$ in contrast only shows an even stronger plateau behavior than the BIC. The $vrEIC_{simple}$ is almost equivalent to $vrEIC_{complex}$. This might be due to the models that generated the data having a very low number of knots.



(a) EIC_{trials} (b) $vrEIC_{trials}$

(c) $EIC_{complex}$ (d) $vrEIC_{complex}$ (e) EIC_{simple} (f) $vrEIC_{simple}$

Figure 5.2.2: The differences in how the different EIC values punish complexity shows very different evaluations. Some (eg. $EIC_{complex}$) find a clear global minimum, others ($vrEIC_{complex}$) see the optimum with having as few splines as possible. EIC_{trials} might even suggest that an even higher complexity might not be detrimental to the model.

5.2.2 Discussion

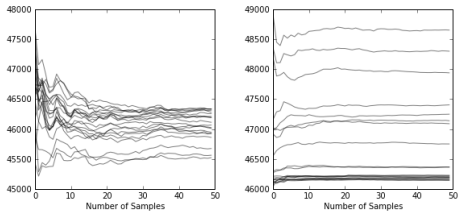
The test likelihood gave a very clear indication when over fitting is occurring, namely after adding more than 100 knots. In the training likelihood this is noticeable by the decreased in incline after 100 knots. This means, that an arbitrary penalty factor α of complexity exists for this particular set of models, such that

$$IC(m, d) = -2 \cdot l(m, d) + \alpha k \tag{5.6}$$

IC is some information criterion, $l(m, d)$ is the log-likelihood of the model, k is the number of parameters.

will give an optimum at the maximal test likelihood. However, this penalty factor might be different for the adaptive rate models and the linearly spaced rate models.

The AIC has a penalty factor of $\alpha = 2$ and finds the optimum of the adaptive rate model. The BIC has a factor of $\alpha = log(3300) = 8.1$ and finds the optimum of the linearly spaced models. This means that a penalty factor multiplied with the complexity of the models might not find both optima at once. An α of 4 might, but this would be an a-posteriori tuning of the parameter without any



(a) $EIC_{complex}$ (b) $vrEIC_{complex}$

Figure 5.2.3: The progression of EIC converging to its value used in Figure 5.2.2. The $vrEIC$ converges quicker, but for the conservative EIC there is not much movement to be expected either.

theoretical justification, purely on the basis on what we know would lead to a good result.

Independent of whether there is or is no optimum of number of knots, we can ask, whether having too few or too many knots will make our model worse. The AIC would say, a small number of knots will give worse models, above 100 they are about equally good, while the BIC would say that below 30 are good models, 50 is even a bit better, but after that the model will be worse by far.

The EIC criteria, eg. the $vrEIC_{trials}$ will give different answers for the adaptive and lin-spaced rate models. For the adaptive rate, higher number of knots are bad[6] (similar to BIC), for the lin-spaced rate, more knots are generally not bad, but also do not improve the model (similar to AIC).

That $vrEIC_{complex}$ and $vrEIC_{simple}$ show no improvement after 30 knots is probably due to their own models having a very low number of knots. Although the $vrEIC_{complex}$ model is named *complex*, it is actually not *that* complex when seen from the perspective of the rate models, which are not interested in crosstalk between the neuron assemblies. However, the $EIC_{complex}$ and EIC_{simple} find an optimum at around 100 knots, which coincides with the test likelihood.

So, somehow the conservative EIC can utilize data fluctuations to estimate a bias that comes close to the test likelihood, while for the $vrEIC$ the difference between fluctuations and the real data create a bias that effectively inverts the training likelihood.

This might be explainable by the uninformative nature of the bootstrap data: The data that was generated by the low-knot-number models did not allow the models to learn about the actual structure of the data, such that even models with a high number of rate knots only emulated the low-knot fluctuations. When compared to the actual model, all models had roughly the same $l(\hat{\mathbf{m}}, d)$, as it - at best - emulated the rate function of the generative model. As the complexity of the model rises, the bias gets larger as the actual model is able to predict the data more accurately, while the bootstrap models remain at some fixed level.

[6] which is plausible, should the adaptive rate component indeed be defective

The bias rises with the likelihood gained on training data, as this is what the $l(\hat{\mathbf{m}}, d)$ term is compared to.

The bias correction of the $EIC_{complex}$ and EIC_{simple} does not contain this large term and is therefore less influenced by the inverse shape of the training likelihood.

Chapter 6

Conclusions

The prospects of using a sampling method to provide an unbiased model evaluation criterion on the basis of training data is promising a lot. If successful, cross-evaluation will no longer be needed and more data can be used for fitting, creating better models. Also an arbitrarily large number of model-selection processes can be included in the fitting process, with each having full access to the data.

But can the methods described in this thesis actually deliver what they promise?

6.1 The Differences between AIC, BIC and EIC

As expected, the AIC bias correction is a very static way to balance complexity of the model. It does not take the data into account or the nature of the components that make the model more complex. From the likelihood on test data, we know that the bias is not static and different models on different data will overestimate its likelihood in differing amounts.

The BIC showed very sparse results for Experiment 1, judging the simpler model a lot better than most other criteria. In Experiment 2 it also penalized the complexity more than the other criteria, which lead to it identifying a potential optimum for the number of knots. However this could also be a false positive. As the trial length gives a large number of observations, the complexity is harshly punished by the BIC[1]. While it was initially only included as the model backends calculated it anyway, it seems an interesting subject for further studies.

For the EIC the outcome relies heavily on what bootstrap transformation is used. Whether data is drawn from the original data, whether as trials or time points, or whether a model was used to create new bootstrap data. Also the two definitions of EIC in Equations 5.4 and 5.5 give different results. In the following sections those options will be compared.

[1] $log(3300) \approx 8.1$, which results in a four times as large bias as the AIC

6.2 The Difference between Conservative and Variance Reduced EIC

While the variance reduced $vrEIC$ can be regarded as a simple extension of the original definition that will converge earlier, Experiment 1 has shown that it also behaves very differently when bootstrap data and real data diverge in their statistics.

It might very well be, that a degenerate transformation of the data (eg. unrelated resampling) will result in a usable conservative EIC, it will certainly give a very intense bias for the variance reduced $vrEIC$. This is because the term to calculate the bias in the conservative Equation only relies on actual data and the term $l(\hat{\mathbf{m}}, \hat{\mathbf{d}}) - l(m, \hat{\mathbf{d}})$ will contain the biased likelihood minus how likely that data is for a normally fitted model.

The inverse term that is used for faster convergence however also includes the likelihood differences on the original data $l(\hat{\mathbf{m}}, d) - l(m, d)$, which for a degenerate model will be far off from the actual model. As the model will generally be better at predicting the actual data, $l(m, d)$ will be closer to 0 than $l(\hat{\mathbf{m}}, d)$. As log-likelihoods are negative, the term $-[l(\hat{\mathbf{m}}, d) - l(m, d)]$ will be very positive, adding to the bias.

The conservative EIC from Equation 5.4 uses the data only to draw biased models from a larger variety of data, while the variance reduced version also uses the greater variance in the reverse term, which makes it essential for the variance reduced version of the EIC, that the actual and the bootstrap data are not too far off.

Also in Experiment 2, the consequences of uninformative bootstrap data could be seen. It will result in the actual model projecting its own training likelihood (including bias) as a bias correction, as the bootstrap models are equally bad at predicting the actual data.

6.2.1 The Difference between Trial Based and Time Based Resampling for EIC

The difference of time based $vrEIC$ and trial based $vrEIC_{trials}$ is not a huge one, as can be expected. A few models may be regarded a tiny bit better by one or the other, but especially for those models, that greatly benefit from a certain connection, this does not interfere at all.

The EIC versions differ a bit more, but also not to an extend that would change the connectivity plots. For cell 4 eg. the EIC_{trials} takes Model 7/4/7 and 7/6/7 to be very close, while EIC, as well as AIC and BIC, see Model 7/4/7 as significantly superior to 7/6/7.

It might be that the EIC did not converge enough for the time point resampling to show meaningful results. All values are fairly close together compared to the variance of the cumulative mean. The inverse term in the $vrEIC$ did, in contrast to the model based resampling, compute a useable bias, excluding 30-50% of the connections. The conservative EIC and EIC_{trials} excluded more

and also differentiated more strongly which model to penalize how strongly. In doing so, it creates a structure that looks very similar to the test likelihood, however the order of the models differs, in some cases severely as some biases are too strong to compensate.

6.2.2 The Differences between EIC with Simple and Complex Models

When data generated by some other model is used as bootstrap data, it is an almost obvious insight that the complexity of the model used for generating the data will have implications for the criterion.

This seems to be true for the variance reduced $vrEIC$ from Equation 5.5, which resulted for the simple model as a no-connections-are-relevant result. For the conservative EIC, the differences are smaller, resulting in almost identical graphs.

When one is interested in the models that are to be compared, as well as how close the data generated by a model is to the original data (as seen by these models), the variance reduced EIC will give valuable insights. But one should keep in mind that the relative complexity differences between generating and evaluated models will not generate a true model evaluation criterion, but rather a comparison given, the data being approximated with a generative model m_g, which model can adapt to variations from the assumed model most effectively. This will always result in models more complex than m_g to be rejected. This can be seen in the simple model for experiment 1 and for both models after a number of knots of 50 in experiment 2.

For the conservative version of the EIC, the choice of the model is less relevant. But for this version even unrelated re-sampled data will give very similar results. The differences between the conservative EIC of the simple model and the AIC in Experiment 1 were not large enough to justify the computational costs, so one might investigate the minute differences further to see how much better the evaluation using the complex model actually are (in the experiment they excluded 7 further connections).

6.2.3 Summary EIC

The two versions, the EIC and the $vrEIC$, show different behavior when the bootstrap data is very unlike the real data. While the EIC is not very interested in the statistics of the bootstrap data, the $vrEIC$ needs a close approximation to produce a meaningful output. Otherwise the $vrEIC$ will simply choose the simplest model, as all others can generalize even worse from the bootstrap data to the real data.

The EIC can work with data a simple model has produced, however it can also work with data that was shuffled such that independent and dependent variables do not match. It remains to be determined whether a bias correction that relies mostly on the model rather than the data, will deliver better or worse results.

6.3 Further Applications of the Toolbox

The **StatCollector** class turned out to be more useful than initially thought. Saving data in a dictionary of dictionaries provided a comfortable level of complexity, such that data generated from parallel run grid processes could be combined effortlessly, yet the relations between the models could be visualized to make informative tree plots.

Also the ability to easily deploy parallel evaluation of models was a necessity to being able to assess the feasibility of different bootstrap model criteria. Using the project infrastructure right now is far from intuitive and might confuse students more than it may help them, but maybe it can be the basis of a future tool to easily distribute computation across the grid.

Overall, the toolbox makes it possible to formulate the creation of models and their application on data in very few lines. The object oriented nature makes it possible to have the data tell you, what can be done with it. Also extending the toolbox with further modular objects is fairly easy.

A rudimentary user manual is included in the appendix, while the full documentation can be accessed via `http://jahuth.github.io/ni/`.

It still remains to be determined what license should be used for the toolbox and how it might be used for teaching in Osnabrück.

Bibliography

[Akaike, 1973] Akaike, H. (1973). Information theory and an extension of the maximum likelihood principle. *Second International Symposium on Information Theory*, pages 267–281.

[Akaike, 1974] Akaike, H. (1974). A new look at the statistical model identification. *Automatic Control, IEEE Transactions on*.

[Costa, 2013] Costa, R. (2013). From Matlab To Python / ni_statmodels repository `https://ikw.uni-osnabrueck.de/trac/ni_statmodelling/`.

[Dayan and Abbott, 2001] Dayan, P. and Abbott, L. (2001). *Theoretical Neuroscience: Computational and Mathematical Modeling of Neural Systems*. Computational Neuroscience Series. Massachusetts Institute of Technology Press.

[Gerhard et al., 2011] Gerhard, F., Pipa, G., Lima, B., Neuenschwander, S., and Gerstner, W. (2011). Extraction of Network Topology From Multi-Electrode Recordings: Is there a Small-World Effect? *Frontiers in computational neuroscience*, 5(February):4.

[Ishiguro et al., 1997] Ishiguro, M., Sakamoto, Y., and Kitagawa, G. (1997). Bootstrapping log likelihood and EIC, an extension of AIC. *Annals of the Institute of Statistical Mathematics*, 49(3):411–434.

[KONISHI and KITAGAWA, 1996] KONISHI, S. and KITAGAWA, G. (1996). Generalised information criteria in model selection. *Biometrika*, 83(4):875–890.

[Konishi and Kitagawa, 2007] Konishi, S. and Kitagawa, G. (2007). *Information criteria and statistical modeling*.

[Perktold et al., 2013] Perktold, J., Seabold, S., Taylor, J., and statsmodels developers (2013). Generalized Linear Models. `http://statsmodels.sourceforge.net/devel/glm.html`.

[Schumacher et al., 2012] Schumacher, J., Haslinger, R., and Pipa, G. (2012). Statistical modeling approach for detecting generalized synchronization. *Phys. Rev. E*, 85:056215.

[scikit-learn developers, 2013] scikit-learn developers (2013). 1.1. Generalized Linear Models - scikit-learn 0.14 documentation. http://scikit-learn.org/stable/modules/linear_model.html#elastic-net.

[Shibata, 1976] Shibata, R. (1976). Selection of the order of an autoregressive model by akaike's information criterion. *Biometrika*, 63(1):117–126.

[van Rossum et al., 2001] van Rossum, G., Warsaw, B., and Coghlan, N. (2001). PEP 8 – Style Guide for Python Code. http://www.python.org/dev/peps/pep-0008/.

List of Figures

6.4 Acronyms

IKW Institut für Kognitionswissenschaft Osnabrück . . . 3

AIC Akaike Information Criterion . . . 5

BIC Bayesian Information Criterion . . . 5

EIC Extended Information Criterion . . . 5

EIC conservative EIC using time reshuffle . . . 3

$vrEIC$ variance reduced EIC using time reshuffle . . . 2

EIC_{trials} conservative EIC using trial reshuffle . . . 45

$vrEIC_{trials}$ variance reduced EIC using trial reshuffle . . . 45

$EIC_{complex}$ conservative EIC using a complex model . . . 46

$vrEIC_{complex}$ variance reduced EIC using a complex model . . . 2

EIC_{simple} conservative EIC using a simple model . . . 46

$vrEIC_{simple}$ variance reduced EIC using a simple model . . . 2

$EIC_{unrelated}$ conservative EIC using unrelated data . . . 47

$vrEIC_{unrelated}$ variance reduced EIC using unrelated data . . . 47

GLM Generalized Linear Model . . . 9

Appendices

Appendix A

Using the Toolbox

A.1 Setting up a the Necessary Python Packages on Your Own Computer

The toolbox needs a range of packages to function properly.

matplotlib	plotting
numpy	matrix calculations
pandas	data frames
scikit learn (sklearn)	models
statmodels	models

Table A.1: Packages needed for running the toolbox

ipython	interactive console and web-based notebooks
sphinx	documentation
guppy	inspection of the program heap

Table A.2: additional packages that are recommended

On most Linux versions there will also be distribution specific packages of the python packages needed. Eg. on ubuntu / debian based distributions you can install all packages with:

```
$ sudo apt-get install ipython-notebook ipython-qtconsole python-
    matplotlib python-scipy python-pandas python-sympy python-nose
```

Another way is to install *easy_install* / *pip*, then run:

```
$ pip install ipython matplotlib scipy numpy pandas scikit-learn
    statsmodels
```

Installing on Windows can be done by simply *Anaconda*[1], which contains

[1] http://continuum.io/downloads

the needed packages and a version of iPython. As a git client on Windows, one can use *TurtoiseGIT*[2], which integrates in the context menu of the explorer.

A.2 Using the iPython Notebooks or Qtconsole

Once installed, you can start the notebook server or the qtconsole either with the created startmenu shortcuts, or start them as arguments to the ipython executable.

You might want to specify the option `--pylab inline` to include plotting functions in the namespace and enable inline display of plots. Alterantively, you can use the *magic* command: `%pylab inline` in a running iPython notebook or qtconsole.

If you need to change the directory to the directory of the toolbox, use cd in the ipython environment:
`cd C:\Users\Where\The\Toolbox\Is`

Alternatively, the shortcut to the Qtconsole and Notebook iPython can be edited to automatically run in the directory of the git repository and load the pylab functions automatically by adding the option: `--pylab inline` to the arguments and change the path where it is executed.

A.3 Setting up a Private Python Environment

Not all computers in the IKW grid run the same software. If one wants to use a specific python version and packages, one needs to install those packages in ones own home directory. Since the home directory lies on a network storage for IKW computers, the packages will be available on all machines.[3]

On a computer in the IKW network that has `virtualenv` installed (eg. the dolly computers), run the following commands:

```
$ cd ~                  # to get to your home directory
$ virtualenv ni_env     # to create a virtual environement in the
    directory ni_env
$ source ni_env/bin/activate
                        # this activates your virtual environment.
                            Everything that is installed now will only
                             be installed for the environment
$ pip install ipython   # to install eg. ipython
$ deactivate            # to close the virtual environment
```

In this virtual environment, every python package can be installed without administratior privileges. But since the home directories are limited in space, it might be wise for a course of students to set up a virtual environment on a network storage. However, this requires either trust in the students, or a fine grained access permission for this directory.

[2] https://code.google.com/p/tortoisegit/

[3] The following method is described in detail in https://ikw.uni-osnabrueck.de/trac/ni_statmodelling/wiki/PythonInstallation in Section University Computers.

A.4 Setting up the Toolbox

The toolbox can be downloaded from `https://github.com/jahuth/ni`. Clone the repository with git or download it as a zip package. Put it either in some directory you will work in, or (for linux) in `/usr/local/lib/python` and/or add its location to your `$PYTHONPATH` by adding the following line to your `~/.profile`:

```
export PYTHONPATH=$PYTHONPATH:/where/you/put/the/toolbox
```

Do NOT include the `ni/` part in the python path. Otherwise you will be able to include the modules **model**, **data** and **tools**, but not **ni**, **ni.model**, etc. The toolbox can not work this way.

A.5 `ssh` and Remote Access to the IKW Network

If one has a user account that is eligable to IKW network access, one can login from anywhere via the `gate.ikw.uos.de` gateway. Since the gateway should not be used to run computation intensive programs, one should connect from there to another computer in the network.

```
user@computer:~$ ssh rzlogin@gate.ikw.uos.de
password:
Welcome! [...]
rzlogin@gate:~$ ssh dolly01.cogsci.uos.de
password:
rzlogin@dolly01:~$ screen bash
rzlogin@dolly01:~$ source ni_env/bin/activate
(ni_env)rzlogin@dolly01:~$
```

It is advisable to use `screen <command>` when connecting from other computers. In case the connection is closed, `screen` will keep the programs running and store the output in its buffer. Further it can open new additional command windows without having to connect to the computer multiple times. To reconnect to a running `screen` session after the connection was closed, `screen` has to be called with the `-r` flag.

`screen` uses Keybindings to open new console windows and switch between them. Pressing `Ctrl + A` and then `Ctrl + C` will create a new window. `Ctrl + A` and then `Ctrl + N` will switch to the next window. For a full explanation, run `man screen` to view the manual pages for the program.

A.5.1 Setting up Public Key Authentification

It is possible to log into `ssh` shells without entering ones user password. Using `ssh-keygen` one can generate a public/private key pair on a local computer. If the public key is added to the `~/.ssh/authorized_keys` file via the command: `ssh-copy-id -i key_file.pub user@gate.ikw.uos.de`

Note that if no passphrase is entered when generating a key, the key will be saved unencrypted and one has to take extra care to secure the private key file from unauthorized access.

Since the home directories in the IKW network are on a network storage, if a key is generated on a IKW computer (and hence saved in `~/.ssh`), and then added to the `~/.ssh/authorized_keys` file, the key can be used to login from any computer in the network to any other.

A.6 Creating a Project

A project can be created wherever one wants. If one plans to use the grid, this should be on a network storage, as the machines that process the computations will need access to it. Also it should not be inside the home directory, if it is expected to output a lot of bootstrap data, as the home directories are restricted in size. However, one can link any directory into ones home directory to have easy access to it.

```
$ cd ~
$ ln -s /net/store/.../ ni
```

Will create a directory link `ni/` in the home directory that contains whatever is in the network storage path.

A project is created by creating a folder containing a `main.py` file. This file can either contain normal python code or python code separated by **job** statements.

To set up a session of waiting jobs, open up the **frontent.py** console by typing:

```
$ ipython frontent.py YourProjectFolder
```

If the folder is not specified or not found, you will be prompted to enter a project path.

Once the project is loaded, you will have a window with a blinking command prompt at the bottom. The topmost line will say something like:

`Project:  YourProjectFolder/ menu`

The second line will say:

```
This project contains no sessions.  Create a session by typing > setup
session
```

Typing into the command prompt `setup session` and pressing enter will ask about some parameters (if a section in the source file is marked accordingly) and on pressing escape run the first part of your `main.py` file to determine how many jobs are to be created. Depending on whether data is loaded, this can take some time. The command prompt is locked until the operation is complete.

The second line should now say:

```
[autorun off] Session:  [0] YourProjectFolder/ sessions/session1/
```

The third line will contain the available information tabs about the session:

```
[ menu ] status jobs pending [120] starting...  running...  done.  failed.
```

Using the arrow keys left and right, the tabs can be changed to the next and previous ones. The Page Up/Down (on German keyboards: Bild Auf/Bild Ab) keys change between sessions, if more than one session is created.

The `status` tab will say that all jobs are currently pending. Typing `run` and pressing enter will run the next available job. Typing `autorun on` and pressing enter will start all available jobs with a delay of one second per job. The maximum amount of jobs running at any time can be configured (see 4.1 and the *help* command of the frontend).

A.6.1 Inspection of Progress

The progress of running jobs can be inspected with the **frontent.py** console, but a better overview about partially computed results is the html output. In the **frontent.py** console with the project selected, run `save project to html` to generate html output for all sessions of this project.

This will create a `project.html` file in the project directory and a `session.html` file in every session directory. These files can be viewed remotely, if connecting via `sftp` to the fileservers of the university (eg. over `gate.ikw.uos.de`).

A.7 Extending the Toolbox

You can easily add new capabilities to the toolbox and even have them included into the main branch. To do so, create a fork (see `https://help.github.com/articles/fork-a-repo`) and/or clone the git repository to somewhere local on your computer:

```
$ cd ~/where_I_want_the_toolbox
$ git clone https://github.com/jahuth/ni.git # or your username
    instead of jahuth
$ cd ni
```

Then add new modules or extend old ones:

```
$ vi ni/data/random.py
```

```
"""
    A module that generates random data for one cell only
"""

import ni.model.pointprocess
import data

def Data(p=0.01,l=1000):
    return data.Data(ni.model.pointprocess.createPoisson(p,l).
        getCounts())
```

(Save by pressing ESC and then type :wq ENTER)

Add your new module to the repository by typing:

```
$ git add ni/data/random.py
```

Then, add the new module to `ni/ni/data/__init__.py`, such that it will be included when `include ni` is called:

```
$ vi ni/data/__init__.py

import data
import monkey
import random
```

Then commit your changes:

```
$ git commit -a -m "Added a new module for random data"
```

If you forked the repository, you are now able to push your changes into your own fork repository and ask a pull-request (or not). If you only cloned the repository, but you would like to see your work in the toolbox, you can generate a patch file and send it via email:

```
$ git format-patch --to jahuth@uos.de HEAD~..HEAD # the character
    after the first HEAD is a tilde
```

HEAD~.HEAD will take into account all changes between your latest version and the latest version that was downloaded by you.