
Monte – machine learning in Python

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Roland Memisevic

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Department of Computer Science
University of Toronto
Email: roland@cs.toronto.edu

Abstract

Monte (Python) is a machine learning framework written in Python. Its purpose is to facilitate the rapid development of gradient-based learning machines, including neural networks, conditional random fields, logistic regression, and others. This document describes the usage and a bit of the design philosophy behind Monte.

This document is currently in the making. If you miss parts of some sections now, there is a good chance that you will find them if you check back tomorrow.

Contents

1	Installation	1
1.1	Getting Monte	1
1.2	Installing Monte	1
2	Using the models	2
2.1	Models and trainers	2
2.2	Example: Constructing a simple conditional random field	2
	Extension to nonlinear conditional random fields	4
3	Assembling models from components	5
3.1	Example: Constructing a linear regression model from scratch	6
	Checking the correctness of the model	7
	Extension to non-linear regression	8
4	Summary of available models	9
5	Future	10
6	License	10

1 Installation

Monte is released under the license described in the file LICENSE, which is part of the Monte distribution.

This section describes where to get, and how to install Monte 0.2.0. If you look ahead, you will notice that this section takes up far less than one page. This is not accidental. Monte 0.2.0 can usually be installed, and is ready-to-use within a few minutes or less.

1.1 Getting Monte

Monte is available at <http://sourceforge.net/projects/montepython/>. To get the most out of Monte, the packages Numpy (Version 1.0 or later), Scipy and Matplotlib (Version 0.87 or later) should to be installed as well – if not present already. Installing those packages is advisable for any serious data-analysis, machine learning, or numerical processing tasks using Python.

1.2 Installing Monte

Installing Monte is very simple: Just copy the main directory `monte/` somewhere into your Python search path. Also make sure that you have the numerical supporting packages listed in the previous section on your path. That's all! You should be ready to use Monte now.

2 Using the models

This section describes how to use and apply models that are defined in Monte.

2.1 Models and trainers

The two most important kinds of object in Monte are *models* and *trainers*. Models are learning machines, and trainers are optimizers that can adapt a model's parameters based on data. The interplay between models, trainers and data is based on a few very simple conventions that we outline in the following.

Models are learning machines, that typically contain parameters. These need to be set based on training data. Examples of models are linear regression, neural networks and logistic regression. While Monte provides these and some other readily defined models, Monte's main goal is to make it easy to build your own models from components. How to define new models using Monte components is described in detail in Section 3. This Section focusses on using existing models, both pre-defined ones and ones that have been built using Monte components.

A model in Monte can be defined as a simple Python class. By convention, model parameters are contained in an attribute called `params`, which is a numpy array of rank 1 (that is, a numpy array whose `shape`-attribute is a tuple of size 1). Trainers access this array in order to adapt the model's parameters (more on this in a moment). Models furthermore contain two methods needed by trainer-objects to optimize the parameters. The method `grad` returns the gradient of the model's objective with respect to its parameters; the method `cost` returns the model's objective function (also a function of the model's parameters). While `params` and `grad` are always expected to be present in a model, the method `cost` is not always present. The reason for this is that there can be models that do not have a well-defined objective function, but that can be trained nevertheless using gradient-dynamics.

The presence of these attributes (member `params`, method `cost`, and possibly method `grad`) is all that is required to define a "model" in Monte's terms. Any class that implements these attributes qualifies as a Monte model and can be trained with a trainer object.

A trainer in Monte is a simple Python class, too. Trainers are used to adapt a model's parameters so as to minimize its cost function. For this purpose, a model is *registered* with a trainer at the time the trainer object is constructed. Trainer objects are expected to take at least one argument in their `__init__`-method – the model that they are supposed to optimize. Most trainers have a `step`-method, which performs a single step of gradient-based optimization. The definition of "a step" can differ from trainer to trainer; it can mean one step of online gradient descent, or one batch of conjugate gradients iterations, for example.

A trainer works by repeatedly calling its model's `cost` and `grad` methods and modifying the model's `params` in order to minimize the model's `cost`. There are no additional rule or conventions that define a proper trainer. However, most trainers are derived from a super-class `Trainer` contained in `monte.train`. That super-class provides some convenience book-keeping that can be useful when defining a trainer.

In the following section we will take a look at an example. We use a readily defined model for this purpose. Most models reside in `monte.models`.

2.2 Example: Constructing a simple conditional random field

To get an idea of how Monte works, we will now take a look at the file `'crf_example.py'` in the subdirectory `'examples'`. The example describes how to build a conditional random field (CRF) from scratch. CRF's are simple probabilistic models for predicting a whole collection of class-labels (a sequence in this case) simultaneously.¹

Let us go through the example in a step-by-step fashion to see what is going on:

```
from numpy import *
from monte.models.crf import ChainCrflLinear #all ready-to-use models
                                              #reside in monte.arch
import monte.train #everything to do with training resides in
                  #monte.gym
```

The file starts with some import statements. Since we will be juggling arrays and numerical objects anyway, we get the all the `numpy` definitions first (lines one and two).

More interesting are lines three and four: In line three we get the class `ChainCrflLinear` from the module `monte.models.crf`. The module `ChainCrflLinear` is one of several modules that live in the sub-package `monte.models`. Some siblings of the module `crf` include, for example, the module `knn`, or the module `autoencoder`. The class `ChainCrflLinear` is all we need from the module for now. It defines a linear chain conditional random field. It contains the methods that are necessary to perform inference or otherwise apply the crf, and holds all the parameters, and settings (such as the number of input-dimensions and number of classes), etc. (We will see how to actually instantiate a `ChainCrflLinear`-object in a moment.)

In line four we import the `train`-module. It contains a set of `trainer`-classes, that can be used to train any system that conforms to the model-conventions described above. Training a model usually amounts to performing some kind of numerical optimization. Since there are many ways of performing such an optimization, there are also many different `trainers`. Note also that, how you *train* a model is typically unrelated to how your model is defined. This is why trainers and model-definitions are kept separately.

The `train`-module contains a set of different trainers (some are good for online-training, some are good for batch-training, some are good for models that don't have an objective function, some are good for other things). We will pick a trainer that's good for our purpose in a moment. First, let us look at the next line:

```
mycrf = ChainCrflLinear(3,2)
```

To instantiate our `ChainCrflLinear`-class, we pass in two parameters: The number of input-dimensions, and the number of classes that each label can take on. These are the only two parameters, that the `ChainCrflLinear`-class expects. To find out how to instantiate some other model, try `help` or take a look at the model-definition.

After instantiating the model, we can construct a trainer for the model. We do so by instantiating one of the `trainer`-classes:

¹We could have used any other kind of model, but CRF's are kind of hot right now... Using another model, say a neural-network regression model, the example would have looked almost the same. You are welcome to try this...

```
mytrainer = monte.train.Conjugategradients(mycrf,5)
```

The trainer `Conjugategradients` uses `scipy`'s conjugate gradients-solver to do the job and is relatively fast. If `scipy` was not available, we could have used a more self-contained trainer, such as `trainer.gradientdescentwithmomentum`, that does not require any external packages.

The constructor for the trainer `Conjugategradients` expects two arguments: The first is the model that we want our trainer to take care of. The second is the number of conjugate-gradient-steps each call of the trainer is supposed to do. While the second argument is specific to this particular type of trainer, the first (the model) is common to all trainers: We need to *register* the model that we want to train with the trainer object. Internally, what this means is that the trainer object receives a pointer to the model's parameter-vector. This parameter-vector is what is being updated during training. The trainer repeatedly calls the model's objective-function, and gradient (if available) to perform the optimization. Other trainer-objects might expect other additional arguments – again, the online-help, or a look at the class-definition, should be consulted to find out which.

To see if the model works at all, let us produce some junk data now:

```
inputs = randn(10,3)
outputs = array([0,1,1,0,0,0,1,0,1,0])
```

We simply produce a sequence of ten three-dimensional random vectors. The `ChainCrfLinear`-class expects the first dimension to be the 'time'-dimension (10 in our case), and the second dimension to be the input-space-dimension (3 in our case). We also produce a sequence of (10) corresponding labels (also random, for the sake of demonstration). The label-sequence is encoded using a rank-1-array. Each single class-label is encoded as an integer, with 0 being the first class. This encoding is a convention that is used by other classification-type models in `monte`, too.

We are now ready to train the model. For this end, all we need to do, is repeatedly call the `step()`-method of the trainer. Since this is just a demonstration, we simply train for 20 steps now. (In a real application, we would probably use a more reasonable stopping criterion, and more reasonable data)

```
for i in range(20):
    mytrainer.step((inputs, outputs), 0.001)
    print mycrf.cost((inputs, outputs), 0.001)
```

We pass two arguments to our trainer's `step()`-method. All the trainer does is, (repeatedly) passing these on to the cost- and gradient functions of the learning machine that we previously registered with it. So it's actually the `ChainCrfLinear`-object that requires two arguments for training. The two arguments are a tuple containing inputs and outputs (we could have passed in a *list* of input-output-pairs, if we had several sequences to train on) and a *weightcost*. Most parametric models in `monte` require a *weightcost* for training. The *weightcost* is a multiplier on a weight-decay term used for regularization.

Finally, we can apply the model on some random inputs. To get the optimal class-labels on the test-inputs, we call the `ChainCrfLinear`'s `viterbi()`-method. (The viterbi-algorithm is what's typically used when classifying with a crf. Many other models, such as regression or simple classification models, have a method `apply()` instead):

```
testinputs = randn(15, 3)
predictions = mycrf.viterbi(testinputs)
print predictions
```

Extension to nonlinear conditional random fields

One benefit of Monte’s modular design is that many of its models can be easily modified or extended in various ways. One way we can modify a crf, for example, is by defining its observation potentials to be a *non-linear* function instead of using the common linear potential function. A model that does this is defined in the class `ChainCrfNNIsl`, which resides in the same module as our chain crf above.

`ChainCrfNNIsl` uses a back-prop-network with one (sigmoid) hidden layer as the observation potential. (Other extensions, such as those that redefine both the observation-potentials and the compatibility-potentials to be non-linear, can be constructed quite easily, as well.) Why the strange name? ‘NNIsl’ means ‘neural network with the structure: inputs–sigmoid–linear’. This kind of abbreviation is used at several places within Monte to denote various types of neural network.

To train and apply this non-linear version of a crf, we can proceed just as we did before. We only need to replace the statement that constructed our linear model previously by one that constructs a non-linear one now:

```
from monte.models.crf import ChainCrfNNIsl
mynncrf = ChainCrfNNIsl(3, 10, 2)
```

The non-linear model expects a number of hidden units as its second argument, which we set to 10 here. We can define a trainer just as before, since training is the same for non-linear and linear models:

```
mytrainer = monte.train.Conjugategradients(mynncrf, 5)
```

To train the model use calls to the trainer’s `step`-method, just as before:

```
mytrainer.step((inputs, outputs), 0.001)
```

3 Assembling models from components

In this Section we take a look at how to assemble your own models using the components that Monte defines.

Monte uses a modular design-philosophy that relies to a large degree on *error back-propagation*. Error back-propagation (often just “back-prop”) is a common algorithm for computing gradients to train learning machines. It was initially invented for neural networks, but back-prop is useful in a much larger context and can be deployed in a wide variety of models. Back-prop learning is especially useful when implemented in an object-oriented language. This observation is the basis for the fantastic back-prop libraries available for the Lush-language² developed by Yann LeCun and Leon Bottou, the main inspiration behind Monte.

The basic idea behind back-prop learning is that it is easy to compute gradients in complicated systems composed of multiple modules, *as long as we can compute gradients of each module with respect to its inputs*. This fact is a simple consequence of the chain rule for differentiation, and it unfolds its full power when combined with object oriented design: As long as we define modules, such that they can compute derivatives with respect to their inputs from derivatives with respect to their outputs, combining them to large, complex systems is simply a matter of sticking the modules together. Just as the outputs of a composed system can be computed as a cascade of function evaluations, gradients are computed simply as a cascade of gradient computations. That is, the chain-rule never needs to be evoked explicitly.

To implement this idea, the back-prop modules in Monte contain four crucial elements, following a similar design in Lush’s back-prop modules:

²<http://lush.sourceforge.net/>

1. An `fprop`-method that computes its outputs from its inputs (short for “forward propagation”),
2. A `bprop`-method that computes the derivatives with respect to its inputs (from derivatives with respect to its outputs; short for “backward propagation”),
3. A `grad`-method that computes the gradient with respect to its own parameters (from its inputs and the derivatives with respect to its outputs)
4. A `params`-attribute that points to the module’s parameters (which are always a rank-1 Numpy-array).

The `fprop`-, `bprop`-, `grad`- and `params`-members can be found in practically every back-prop-module defined in Monte. All back-prop modules are defined in the package `monte.models.backprop`. Most back-prop modules also contain a convenience-function called `numparams`, that computes the number of parameters that the module requires (and thus the length of its parameter-array).

Given a back-prop model and some data, computing gradients for all modules contained in the system follows basically always the same procedure: We first compute a “forward-pass” by calling the modules’ `fprop`-methods. If our system is composed of multiple modules, the outputs of one module will be the inputs of one or more other modules. The final module is often one that computes a cost, such as a squared reconstruction error.

After computing the forward-pass, we compute a “backward-pass” by computing all modules’ `bprop`-methods to obtain derivatives with respect to their inputs. To do so, we need to reverse the order of calls that we used for the forward-pass: This will make sure that a successor-module’s input-derivatives will be used by the predecessor-module as output-derivatives – from which the predecessor computes its own inputs-derivatives, which become it’s own predecessor’s outputs, etc.

Finally, after we completed the backward-pass, we can get each module’s parameter-gradients by calling their `grad`-methods. The following code-snippet demonstrates this idea. It defines a complete, self-contained class (a model for performing linear regression), that could be readily trained with a `trainer`-object and applied to some real data:

3.1 Example: Constructing a linear regression model from scratch

```
from numpy import hstack
from numpy.random import randn
from monte.models import backprop

class LinearRegression(object):
    """A simple linear regression class built with Monte back-prop
    components.
    """

    def __init__(self, numin, numout):
        self.numin = numin
        self.numout = numout
        self.params = 0.01 * randn(backprop.neuralnet.Linearlayer.numparams(numin, numout))
        self.functionmodule = backprop.neuralnet.Linearlayer(numin, numout, self.params)
        self.costmodule = backprop.cost.Squarederror()

    def cost(self, inputs, outputs):
        return self.costmodule.fprop(self.functionmodule.fprop(inputs), outputs)

    def grad(self, inputs, outputs):
        modeloutputs = self.functionmodule.fprop(inputs)           #forward pass
        self.costmodule.fprop(modeloutputs, outputs)               #...
        d_outputs = self.costmodule.bprop(modeloutputs, outputs)  #backward pass
        self.functionmodule.bprop(d_outputs, inputs)               #...
        return self.functionmodule.grad(d_outputs, inputs).sum(1) #compute gradient

    def apply(self, inputs):
        return self.functionmodule.fprop(inputs)
```

Let us go through the code step by step to see how it implements the strategy described above:

As mentioned in the previous section, any ready-to-train model should be a Python-class that contains at least a `cost`- and a `grad`-method. Our model makes use of back-prop-learning to implement both of these as we describe in detail in a moment. Note, that the model also defines an `__init__` and an `apply`-method for convenience of use.

The `__init__`-method contains some boilerplate. It initializes the model by (i) saving the number of input- and output-dimensions (lines 1 and 2 of the method), (ii) making a parameter-array, filled with some small random values using Pylab's `randn`-function (line 3) and (iii) constructing the two back-prop modules, that our model is supposed to use: One for computing a linear regression function and one for computing a reconstruction-cost (lines 4 and 5). The linear regression function is taken from `backprop.neuralnet`. which contains various components useful in building neural networks. Here, we just use the class `Linearlayer` from that module, which computes a simple (affine-)linear function. The cost module is taken from `backprop.cost`.

One very important lesson to be learned from this example is the following: The model's parameters (which, as mentioned above, are saved in a `numpy`-array) belong to the *model*. The model's back-prop modules, in turn, get to see only *pointers* to this parameter-array. And they receive these pointers at the time they are constructed (line 4 in the example). Most back-prop modules expect a pointer to a parameter-array in their constructor³. Later, we will show how back-prop modules can be defined recursively by nesting back-prop modules inside other back-prop-modules. It is important to keep in mind that in cases like these, owner-ship of the parameter-array always stays with the *outer-most*

³The fact that pointers, rather than copies, of the model's parameters are being passed to back-prop-modules is crucial for learning, but happens somewhat unobtrusively and implicitly, by making use of the fact that in Python function calls are by reference.

component. All sub-components receive only references to these parameters. In our case, the outer-most component is our `LinearRegression`-class.

The other back-prop component that our class uses (`backprop.cost.Squarederror`) does not take any parameters. It does compute gradients with respect to its inputs nevertheless – these are always needed for computing gradients further down.

The heart of our `LinearRegression`-class are the `cost`- and `grad`-methods. They are the methods that actually implement the fprop/bprop-scheme described above. The `cost`-method is straightforward. It simply computes a short cascade of the fprop-methods on its back-prop components: Its function-module's `fprop` computes a linear function, its cost-modules `fprop` subsequently computes the resulting squared reconstruction error.

To compute gradients, we need to do a forward-pass followed by a back-ward pass, which is what the `grad`-method does⁴: It first computes the linear function to obtain the model's guess as to what the correct outputs on the given inputs are, followed by the cost-function. It saves the model-outputs in the variable `modeloutputs` (rather than returning it like the `cost`-method). Saving the model-outputs is necessary, because we need them for the backward-pass.

The backward-pass follows right after we computed the forward-pass and calls the model's back-prop components in reversed order: First, we call the cost-modules' `bprop`-method. This method expects the same arguments as the corresponding `fprop`-call: The model-outputs and the desired (training) outputs. This is why we saved the model-outputs before. The modules' output is the derivative of the module with respect to its inputs (which in our case are the model-outputs). We save these derivatives in a variable `d_outputs`. Given the derivatives we can continue with the next module in the backward-cascade: We call our function-modules `bprop`-method using `d_outputs` and this modules' inputs as arguments, and the back-ward pass is completed.

After completing the backward-pass we can call each module's `grad`-method to obtain their gradients. Note, that the only module containing any parameters in our case is the function module. We compute it's gradient (last line in `grad`) and sum it up over all input-cases, which we assume to be arranged columnwise in the input. Since this is the only set of parameters that we use, we directly return the gradient. In case we had several modules with parameters, we would first stack them into a single array. We will see an example of this below.

To complete our `Linear Regression` class we add an `apply`-method for convenience. This method simply applies the learned function to new inputs by calling the function-components `fprop`-method. The result is a self-contained linear regression class that we could register with a trainer and train and apply to real data. In practice we might want to add a regularization term, for example a weight-decay, to the cost function and to its gradient. This is straightforward, and we leave it as an exercise.

Note that in our example we never needed to explicitly compute any derivatives ourselves. While computing derivatives would have been easy in this simple case, the possibility of assembling models from components without needing to calculate any derivatives by hand will become extremely useful as soon we transition to more complex models.

Checking the correctness of the model

As a sanity check, to see whether the model does the right thing, let us compare the parameters it comes up with after training to those that we obtain from using a more traditional approach to doing linear regression.

A more “traditional” way of performing linear regression is by minimizing squared reconstruction error using a closed form solution. Say, we want to apply a model with 5-dimensional inputs and 1-dimensional outputs and we have (columnwise) training data matrices X and Y for inputs and outputs, respectively. Here X is a $5 \times N$ - and Y is a $1 \times N$ -matrix, where N is the number of training cases. Generating some random data could be done like this:

⁴Note that `grad` repeats the forward-pass that `cost` computes. If we can make sure that the trainer that we use to train the model always calls `cost` before it calls `grad`, then we can also do without the forward-pass in `grad`. We shall discuss this topic in more detail later.


```

>>> X = randn(5, 1000)           #create 1000 inputs
>>> w = randn(5)                 #create a linear model
>>> w
array([-0.56883823, -1.47482531,  1.21239073, -1.79361343, -0.64315871])

>>> Y = dot(w, X) + randn(1, 1000) #create the outputs

```

It is well-known that the optimal (in terms of squared error) linear function based on the training data has parameters $w^{\text{linreg}} = (X X^T)^{-1} X Y^T$. In Python, we can write this as

```

>>> dot(inverse(dot(X,X.T)), dot(X,Y.T)).T
array([[ -0.55389647, -1.52445261,  1.17153374, -1.83514791, -0.68079122]])

```

We see that the solution is fairly similar to the actual parameters w . Now, to train our back-prop-module, we can proceed as usual, by instantiating it, building a trainer and running it for a few steps:

```

>>> model = LinearRegression(5,1)
>>> trainer = monte.train.Conjugategradients(model, 20)
>>> trainer.step((X,Y), 0.0)

```

Let us look at the model parameters to check what they look like after training:

```

>>> model.params
array([ -0.55376029, -1.52260298,  1.16934185, -1.83290113, -0.68340035,
        -0.0762695  ])

```

We see that the parameters are very similar to what the closed-form solution gives us. The model parameters have one extra component, which is close to zero, and represents the affine part of the model. (To access the linear part w of our model we could have also made use of the fact that it is exposed as a member `w` by the `Linearlayer`. The affine part is exposed as the member `b`.)

Why doing linear regression in this involved back-prop-way in the first place, given that we can get the solution from a one-liner? One reason is that with the linear back-prop model in place, we are just a stone's throw away from much more powerful (for example, non-linear or multi-layer) models, as we describe in the next section.

Extension to non-linear regression

The modularity makes it trivially easy to extend the model in order to obtain, for example, a non-linear version. Let us consider a non-linear regression model using a simple multi-layer neural network, for example. What we need to do is replace the linear function-module with a non-linear, neural network-based one. The back-prop component `SigmoidLinear` has an interface that is almost exactly the same as the `Linearlayer`-component which we used before. The only difference is that at construction-time the component expects one additional argument, which is the number of units in its hidden layer. To use this component all we need to do is change a few lines in `__init__`. The `cost`- and `grad`-methods stay exactly the same, because all the interfaces are the same. The new `__init__`-method needs to take an additional argument (the number of hidden units) and replace the functionmodule with `SigmoidLinear`:

```

class NonlinearRegression(object):
    """A simple non-linear regression class built with Monte back-prop
    components.
    """

    def __init__(self, numin, numhid, numout):
        self.numin = numin
        self.numhid = numhid
        self.numout = numout
        self.params = 0.01 * randn(backprop.neuralnet.SigmoidLinear.numparams(
                                                    numin, numhid, numout))
        self.functionmodule = backprop.neuralnet.SigmoidLinear(
                                                    numin, numhid, numout, self.params)
        self.costmodule = backprop.cost.Squarederror()

        #rest exactly the same as for LinearRegression

```

It is interesting to note that `SigmoidLinear` is itself composed of multiple sub-components, and it uses its component's forward- and backward propagation methods to do its work. (If interested, take a look at its definition in `'monte/models/backprop/neuralnet.py'`.) However, since gradient-computations are always encapsulated within each component, so we do not need to worry about them, when using the components.

In a similar fashion, we could use a three-layer network or any other type of component to define the function-module.

4 Summary of available models

This section provides a short summary of the currently available models in Monte.

Most of the learning methods are, similarly as the `crf`-example in the previous section, based on parametric models. There are a few exceptions, for example, `k`-nearest neighbors or `k`-means, which contain their own specialized training methods (if any). (See below for details on these and other models).

For the parametric models training has been deliberately separated from the definition of the models themselves. The reason is that training often amounts to performing some form of numerical optimization, and there are many possible ways of performing such an optimization. Which way is the best depends heavily on the application domain and other factors that are completely independent of the model itself. Furthermore, optimization is an 'orthogonal' line of research, and there might be optimization approaches of which we don't even know yet.

The Monte 0.2.0 directory layout is fairly simple. The main directory `'monte/'` contains the following few modules and sub-packages (NOTE: The directory layout changed in 0.2.0 and is not compatible with earlier versions.)

Monte 0.2.0 Directory layout

Directory	Purpose
models/	Sub-package containing all ready-to-use models. Many (but not all) of these models have a grad- and a cost-method. These models can be trained with trainer-objects. Many models are composed of back-prop-components (see below).
models/backprop/	Sub-package containing trainable 'back-prop'-components, the building blocks for gradient-based learning machines. Each back-prop component contains an fprop-method, a bprop-method, and a grad-method. Training of the components is done with error back-propagation. The method fprop computes the response of the component wrt. its input. The method bprop computes the derivative of an error-function with respect to the component's inputs, using the derivative wrt. to it's own outputs. The method grad computes the derivative of the error wrt. the component's parameters. Backprop-components are typically not used as trainable machines themselves. Rather, multiple back-prop components can be combined into models (which reside in the subpackage models).
train.py	The definition of models and of mechanisms for training these is deliberately separated in Monte. The module trainers contains trainer-classes that can be used to train the models. Models are registered with trainer objects at the time the trainer objects are constructed. Training is then performed by repeatedly calling a trainer's step()-method.
examples/	Contains simple example-scripts, that illustrate various aspects of Monte.
util.py	The util module contains utility functions- and classes, such as fuctions for normalizing data, computing 'logsumexp' functions, etc.
doc/	Documentation.

5 Future

6 License

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