Neural Nets with Automatic Differentiation

https://github.com/brunjlar/neural

About Me

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Agenda

- Artificial Neural Networks
- Gradient Descent
- Backpropagation
- The **neurals** library
  - Automatic Differentiation
  - Components
  - Layers
  - Pipes
  - Other Features
  - Examples
- Questions & Comments

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The neural package

[Tags:benchmark, library, mit, program, test]

The goal of neural is to provide a modular and flexible neural network library written in native Haskell.

Features include

- *composability* via arrow-like instances and pipes,
- *automatic differentiation* for automatic gradient descent/ backpropagation training (using Edward Kmett's fabulous ad library).

The idea is to be able to easily define new components and wire them up in flexible, possibly complicated ways (convolutional deep networks etc.).

Three examples are included as proof of concept:

- A simple neural network that approximates the sqrt function on [0,4].
- A slightly more complicated neural network that solves the famous Iris flower problem.
- A first (still simple) neural network for recognizing handwritten digits from the equally famous MNIST database.

The library is still very much experimental at this point.

on Hackage...

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on Hackage...

...and GitHub

Artificial Neural Networks

Artificial Neural Networks
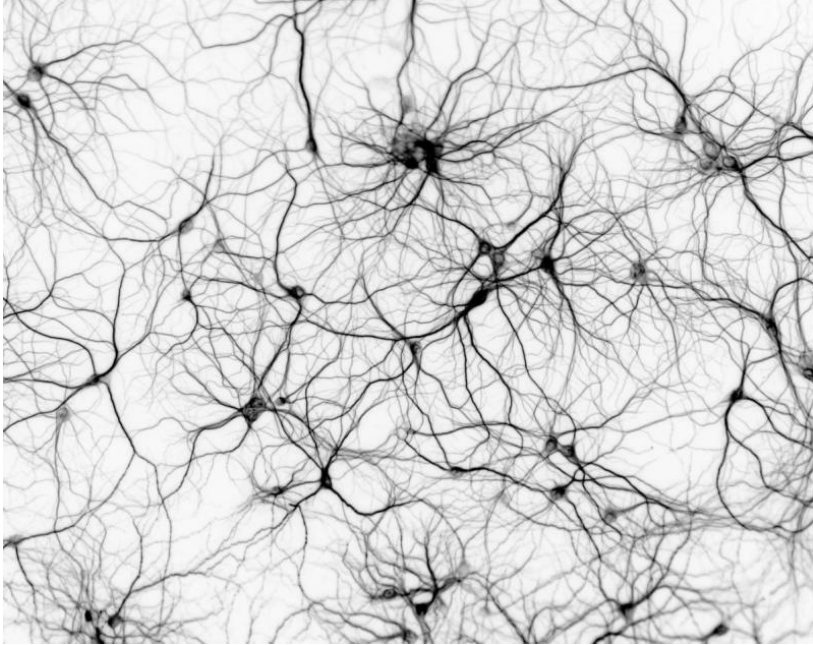
Taking inspiration from biological brains to approach Artificial Intelligence.

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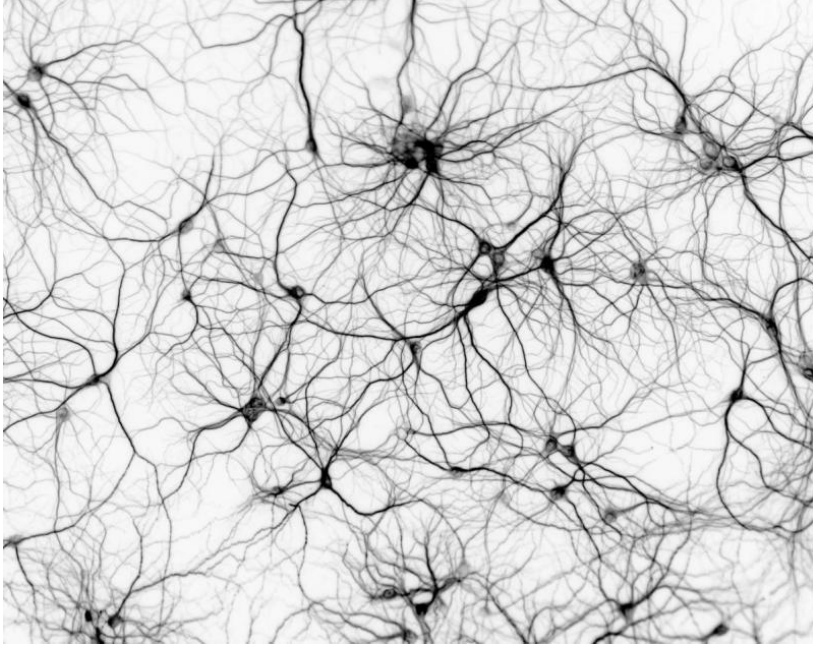
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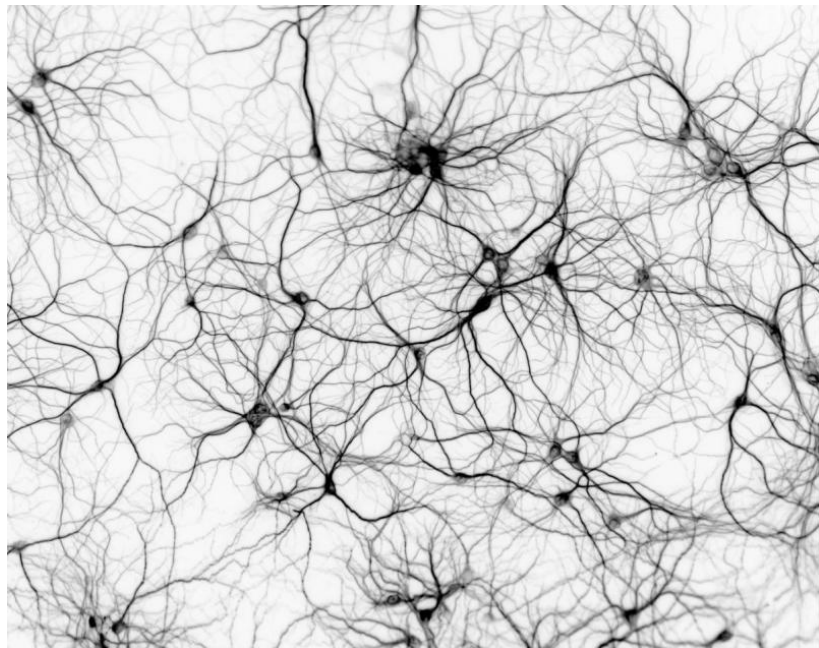
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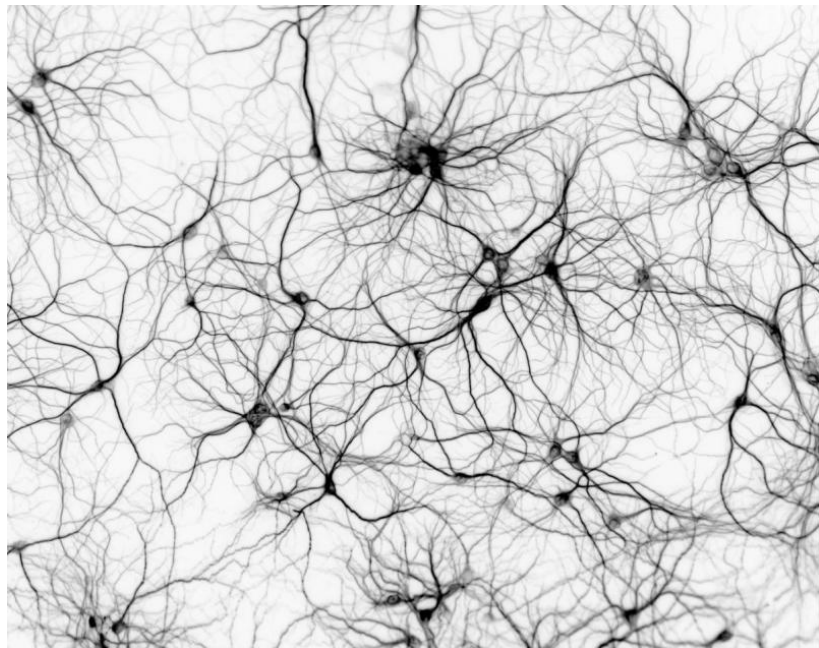
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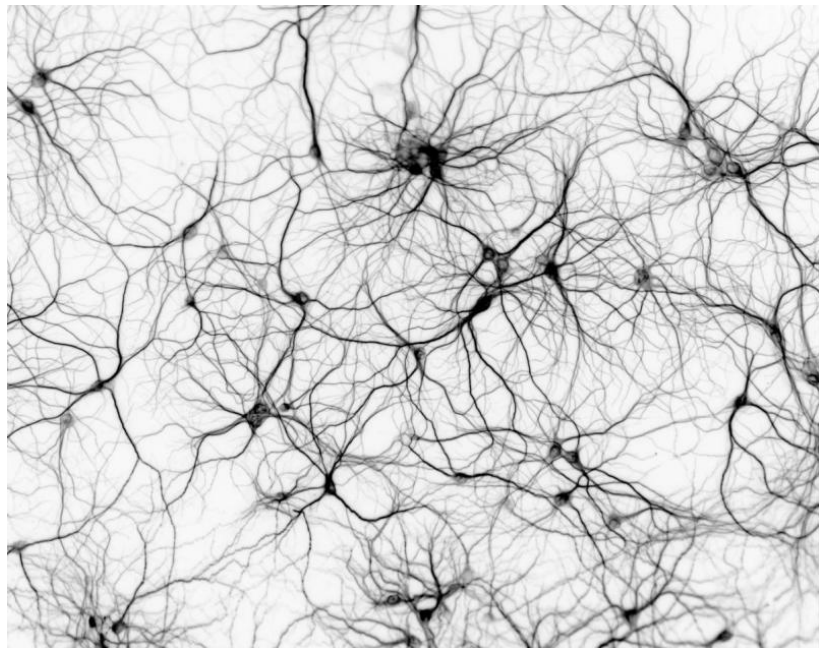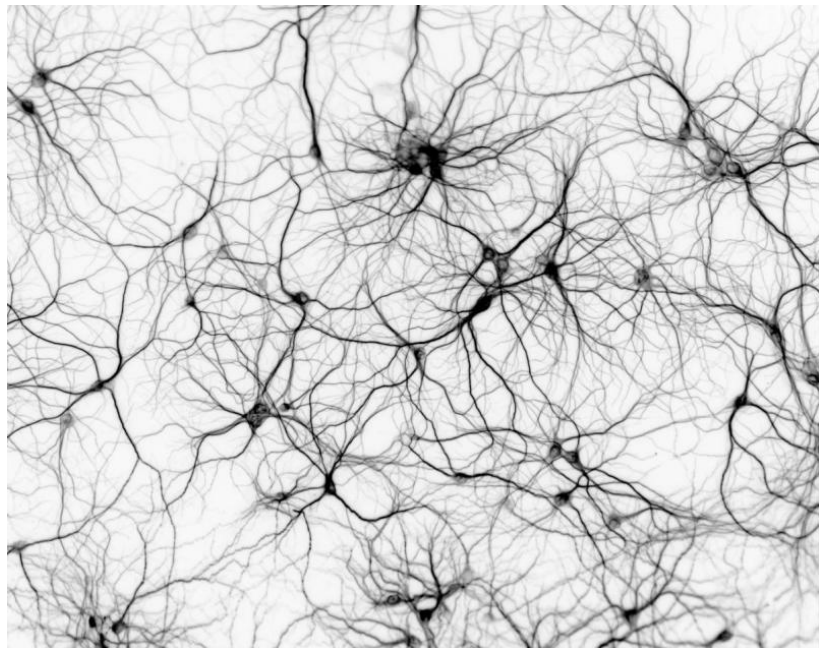

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- 1943 McCulloch-Pitts Neuron

- 1958 Perceptron

- 1975 Backpropagation

- 2006 Deep Learning

- 2015 AlphaGo

Artificial Neural Networks

$$w_{i1}$$

$$w_{i2}$$

$$w_{i3}$$

$$\Sigma \quad f$$

$$\cdots$$

$$y_i = f(net_i)$$

Artificial Neural Networks

$y_i = f(net_i)$

Schematic Diagram of a Neural Network

Input Units   Hidden Units   Output Units

Flow of Activation
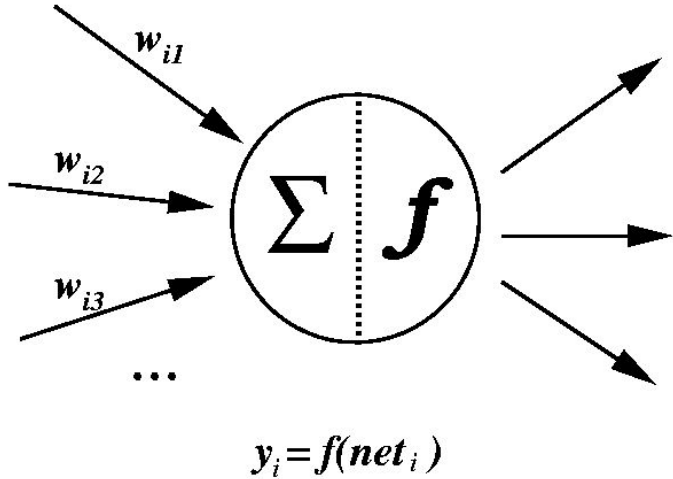
Gradient Descent

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Extremely generic method for finding minima (or maxima) of differentiable functions:

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We want to **minimize** the **error** of our artificial neural networks!

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- The "gradient" points into the direction of steepest incline. $\nabla f = \left(\frac{\partial f}{\partial x_i} \right)_i$

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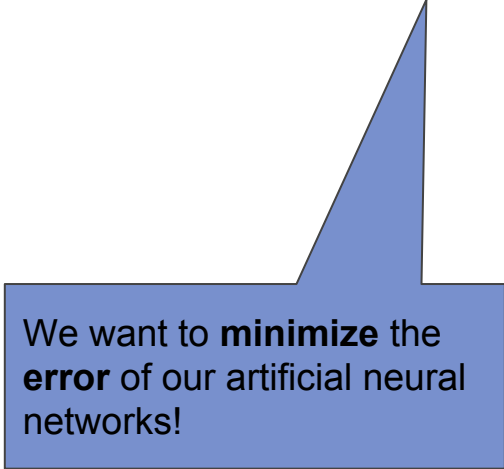
Gradient Descent

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- At each step, move into the opposite direction.

- Eventually, you'll end up at a (local) minimum.

All we need is to compute the gradient!

Backpropagation

Backpropagation...

$$\delta_{Mi} = -\frac{\partial E_p}{\partial O_{pi}} \frac{\partial Y_{Mi}}{\partial net_{Mi}} \tag{2.5}$$

$$\frac{\partial E_p}{\partial Y_{ji}} = \frac{\partial E_p}{\partial net_{(j+1)1}} \frac{\partial net_{(j+1)1}}{\partial Y_{ji}} + \frac{\partial E_p}{\partial net_{(j+1)2}} \frac{\partial net_{(j+1)2}}{\partial Y_{ji}} + \dots$$

$$= \sum_{a=1}^{N_{j+1}} \left[\frac{\partial E_p}{\partial net_{(j+1)a}} \frac{\partial net_{(j+1)a}}{\partial Y_{ji}} \right] \tag{2.11}$$

$$= \sum_{a=1}^{N_{j+1}} \left[-\delta_{(j+1)a} \frac{\partial}{\partial Y_{ji}} (W_{(j+1)a0} Y_{j0} + \dots + W_{(j+1)ai} Y_{ji} + \dots) \right] \tag{2.12}$$

$$= \sum_{a=1}^{N_{j+1}} \left[-\delta_{(j+1)a} \frac{\partial}{\partial Y_{ji}} (W_{(j+1)ai} Y_{ji}) \right] \tag{2.13}$$

$$= \sum_{a=1}^{N_{j+1}} \left[-\delta_{(j+1)a} W_{(j+1)ai} \right] . \tag{2.14}$$

$$\frac{1}{2} \left[(T_{p1} - O_{p1})^2 + \dots + (T_{pi} - O_{pi})^2 + \dots \right] \frac{\partial}{\partial net_{Mi}} f(net_{Mi}) \tag{2.6}$$

$$f'(net_{Mi})$$

$$[f(net_{Mi})][1 - f(net_{Mi})]$$

$$= (T_{pi} - O_{pi})(O_{pi})(1 - O_{pi})$$

$$\delta_{ji} = -\sum_{a=1}^{N_{j+1}} \left[-\delta_{(j+1)a} W_{(j+1)ai} \right] \frac{\partial Y_{ji}}{\partial net_{ji}} \tag{2.10}$$

$$= Y_{ji}(1 - Y_{ji}) \sum_{a=1}^{N_{j+1}} \left[\delta_{(j+1)a} W_{(j+1)ai} \right] \tag{2.16}$$

$$\tag{2.8}$$

...is just Gradient Descent

Mathematically simple, a rather tedious application of the Chain Rule.

Backpropagation

But details change when...

Backpropagation

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- A different activation function is used for neurons.

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Backpropagation

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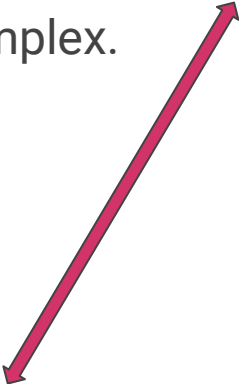
Backpropagation

Furthermore, the classical formulas are **index-based**, i.e. complicated when network topologies become complex.

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$$\nabla f = \left(\frac{\partial f}{\partial x_i} \right)_i$$

Automatic Differentiation

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Less well known is the third way, **Automatic Differentiation** (see Conal M. Elliott's fantastic paper "Beautiful Differentiation"), an **exact numeric** method.

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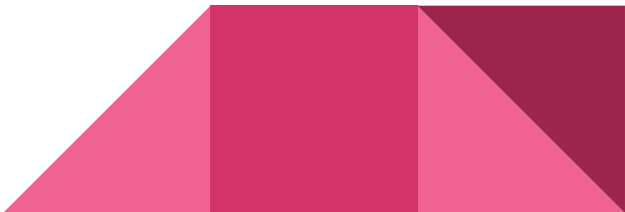
Basic Idea: Manipulate numbers and their derivatives simultaneously (can be done conveniently in Haskell by overloading the numeric type classes).

Edward Kmett's *ad* Library

```haskell
grad :: (Traversable f, Num a) => (forall s. Reifies s Tape => f (Reverse s a) -> Reverse s a) -> f a -> f a
                                                                                                    # Source
```

The grad function calculates the gradient of a non-scalar-to-scalar function with reverse-mode AD in a single pass.

```haskell
>>> grad (\[x,y,z] -> x*y+z) [1,2,3]
[2,1,1]
```

```haskell
grad' :: (Traversable f, Num a) => (forall s. Reifies s Tape => f (Reverse s a) -> Reverse s a) -> f a -> (a,
f a)                                                                                                 # Source
```

The grad' function calculates the result and gradient of a non-scalar-to-scalar function with reverse-mode AD in a single pass.

```haskell
>>> grad' (\[x,y,z] -> x*y+z) [1,2,3]
(5,[2,1,1])
```

```haskell
gradWith :: (Traversable f, Num a) => (a -> a -> b) -> (forall s. Reifies s Tape => f (Reverse s a) -> Reverse
s a) -> f a -> f b                                                                                  # Source
```

grad g f function calculates the gradient of a non-scalar-to-scalar function f with reverse-mode AD in a single pass. The gradient is combined element-wise with the argument using the function g.

```haskell
grad == gradWith (_ dx -> dx)
id == gradWith const
```

```haskell
gradWith' :: (Traversable f, Num a) => (a -> a -> b) -> (forall s. Reifies s Tape => f (Reverse s a) ->
Reverse s a) -> f a -> (a, f b)                                                                     # Source
```

grad' g f calculates the result and gradient of a non-scalar-to-scalar function f with reverse-mode AD in a single pass the gradient is combined element-wise with the argument using the function g.

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grad :: (Traversable f, Num a) => (forall s. Reifies s Tape => f (Reverse s a) -> Reverse s a) -> f a -> f a
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                                                                                          # Source
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                                                                                          # Source
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grad' g f calculates the result and gradient of a non-scalar-to-scalar function f with reverse-mode AD in a single pass the gradient is combined element-wise with the argument using the function g.

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```

Arguments of "traversable" shape - no indices needed!

Edward Kmett's *ad* Library

```
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                                                                                              # Source
```
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>>> grad (\[x,y,z] -> x*y+z) [1,2,3]
[2,1,1]
```

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                                                                                              # Source
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                                                                                              # Source
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grad' g f calculates the result and gradient of a non-scalar-to-scalar function f with reverse-mode AD in a single pass the gradient is combined element-wise with the argument using the function g.

```
grad' == gradWith' (_ dx -> dx)
```

Arguments of "traversable" shape - no indices needed!

These types look intimidating...

Neural Wrapper around *ad*

```haskell
class (Floating a, Ord a) => Analytic a where
```

Class `Analytic` is a helper class for defining differentiable functions.

Minimal complete definition

```haskell
fromDouble
```

Methods

```haskell
fromDouble :: Double -> a
```

⊟ Instances

```haskell
⊞ Analytic Double                                │ # Sou
⊞ Reifies * s Tape => Analytic (Reverse s Double) │ # Sou
```

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Minimal complete definition

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```

Methods

```
fromDouble :: Double -> a
```

Instances

```
Analytic Double                              # Sou
Reifies * s Tape => Analytic (Reverse s Double)  # Sou
```

There are those scary types again!

Neural Wrapper around *ad*

```
newtype Diff f g
```

Type `Diff f g` can be thought of as the type of "differentiable" functions `f Double -> g Double`.

Constructors

```
Diff
    runDiff :: forall a. Analytic a => f a -> g a
```

⊟ Instances

⊞ `Category (* -> *) Diff` │ # Source

```
type Diff' = forall a. Analytic a => a -> a
```

Type `Diff'` can be thought of as the type of differentiable functions `Double -> Double`.

Neural Wrapper around *ad*

gradWith'

`:: Traversable t`	
`=> (Double -> Double -> a)`	how to combine argument and gradient
`-> Diff t Identity`	differentiable function
`-> t Double`	function argument
`-> (Double, t a)`	function value and combination of argument and gradient

Computes the gradient of an analytic function and combines it with the argument.

```
>>> gradWith' (\_ d -> d) (Diff $ \[x, y] -> Identity $ x * x + 3 * y + 7) [2, 1]
(14.0,[4.0,3.0])
```

Components

Components

```
newtype ParamFun s t a b                                    # Sou
```

The type ParamFun s t a b describes parameterized functions from a to b, where the
parameters are of type t s. When such components are composed, they all share the *same*
parameters.

Constructors

ParamFun

```
runPF :: a -> t s -> b
```

⊟ **Instances**

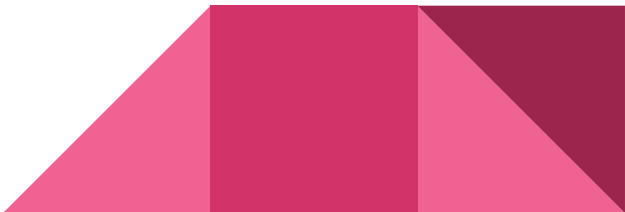| ⊞ Category * (ParamFun s t) | # Source |
⊞ Arrow (ParamFun s t)	# Source
⊞ ArrowChoice (ParamFun s t)	# Source
⊞ Profunctor (ParamFun s t)	# Source
⊞ ArrowConvolve (ParamFun s t)	# Source
⊞ Functor (ParamFun s t a)	# Source
⊞ Applicative (ParamFun s t a)	# Source

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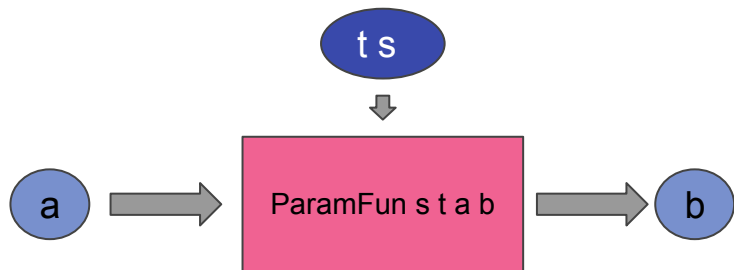
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⊞ Applicative (ParamFun s t a)   # Source

t s

a → ParamFun s t a b → b

Components

```
data Component f g                                                    # Sour
```

A Component f g is a parameterized differentiable function f Double -> g Double. In contrast to ParamFun, when components are composed, parameters are not shared. Each component carries its own collection of parameters instead.

Constructors

```
(Traversable t, Applicative t, NFData (t Double)) => Component
```

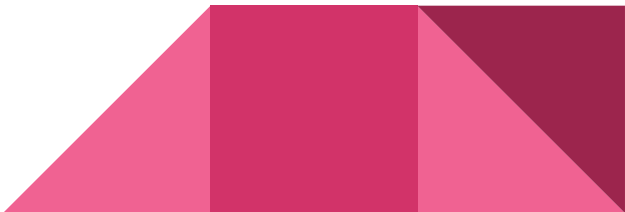|	
`weights :: t Double`	the specific parameter values
`compute :: forall s. Analytic s => ParamFun s t (f s) (g s)`	the encapsulated parameterized function
`initR :: forall m. MonadRandom m => m (t Double)`	randomly sets the parameters

⊟ **Instances**

⊞ NFData (Component f g)	# Source
⊞ Category (* -> *) Component	# Source

Components

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data Component f g                                                          # Sourc
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⊟ **Instances**

⊞ `NFData (Component f g)`	# Source
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The traversable type t is "hidden" by existential quantification

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Constructors

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(Traversable t, Applicative t, NFData (t Double)) => Component
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weights :: t Double	the specific parameter values
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⊟ **Instances**

```
⊞ NFData (Component f g)        # Source
```

```
⊞ Category (* -> *) Component   # Source
```

Traversables are composed automatically!

The traversable type t is "hidden" by existential quantification

Components

```
data Model :: (* -> *) -> (* -> *) -> * -> * -> * -> * where                                                          # Source
```

A `Model` f g a b c wraps a `Component` f g and models functions b -> c with "samples" (for model error determination) of type a.

Constructors

```
Model :: (Functor f, Functor g) => Component f g -> (a -> (f Double, Diff g Identity)) -> (b -> f Double) -> (g Double -> c) -> Model f g a b c
```

⊟ **Instances**

⊞ `Profunctor (Model f g a)` | # Source

⊞ `NFData (Model f g a b c)` | # Source

Components

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data Model :: (* -> *) -> (* -> *) -> * -> * -> * -> * where                                    # Source
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   `Model :: (Functor f, Functor g) => Component f g -> (a -> (f Double, Diff g Identity)) -> (b -> f Double) -> (g Double -> c) -> Model f g a b c`

  ⊟ **Instances**

   ⊞ `Profunctor (Model f g a)` | # Source

   ⊞ `NFData (Model f g a b c)` | # Source

```
type StdModel f g b c = Model f g (b, c) b c
```

   A type abbreviation for the most common type of models, where samples are just input-output tuples.

```
mkStdModel :: (Functor f, Functor g) => Component f g -> (c -> Diff g Identity) -> (b -> f Double) -> (g Double -> c) -> StdModel f g b c
```

   Creates a `StdModel`, using the simplifying assumtion that the error can be computed from the expected output allone.

Components

```
descent

:: Foldable h
=> Model f g a b c          the model whose error should be decreased
-> Double                   the learning rate
-> h a                      a mini-batch of samples
-> (Double, Model f g a b c)  returns the average sample error and the improved model
```

Performs one step of gradient descent/ backpropagation on the model,

Layers

Layers

```
type Layer i o = Component (Vector i) (Vector o)
```

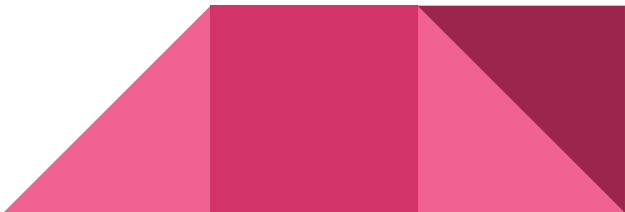A Layer i o is a component that maps a Vector of length i to a Vector of length o.

```
linearLayer :: forall i o. (KnownNat i, KnownNat o) => Layer i o
```

Creates a *linear* Layer, i.e. a layer that multiplies the input with a weight Matrix and adds a bias to get the output.

Random initialization follows the recommendation from chapter 3 of the online book Neural Networks and Deep Learning by Michael Nielsen.

```
layer :: (KnownNat i, KnownNat o) => Diff' -> Layer i o
```

Creates a Layer as a combination of a linear layer and a non-linear activation function.

Layers

```
tanhLayer :: (KnownNat i, KnownNat o) => Layer i o
```
This is a simple Layer, specialized to tanh-activation. Output values are all in the interval [-1,1].

```
tanhLayer' :: (KnownNat i, KnownNat o) => Layer i o
```
This is a simple Layer, specialized to a modified tanh-activation, following the suggestion from Efficient BackProp by LeCun et al., where output values are all in the interval [-1.7159,1.7159].

```
logisticLayer :: (KnownNat i, KnownNat o) => Layer i o
```
This is a simple Layer, specialized to the logistic function as activation. Output values are all in the interval [0,1].

```
reLULayer :: (KnownNat i, KnownNat o) => Layer i o
```
This is a simple Layer, specialized to the *rectified linear unit* activation function. Output values are all non-negative.

Plumbing with Pipes

Pipes API

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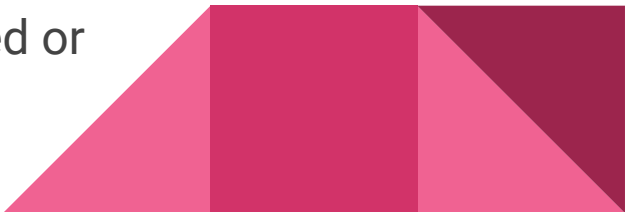
but not enough:

- Training "batches" must be provided - for realistic problems, not all training data will fit into memory.

- We want some progress reporting to see how training is going.

- We want to stop training when some target is reached or no further improvement seems likely.

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All this tends to produce imperative and non modular code…
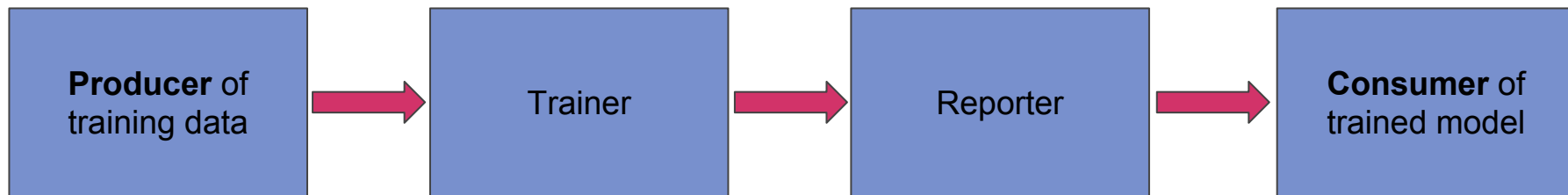
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Pipes to the rescue!

Pipes API

Producer of training data → Trainer → Reporter → **Consumer** of trained model

Pipes API

```
data TS f g a b c                                         # Source
```

The training state of a model.

Constructors

TS

tsModel :: Model f g a b c	updated model
tsGeneration :: Int	generation
tsEta :: Double	learning rate
tsBatchError :: Double	last training error

```
descentP                                                  # Sourc
```

:: (Foldable h, Monad m)	
=> Model f g a b c	initial model
-> Int	first generation
-> (Int -> Double)	computes the learning rate from the generation
-> Pipe (h a) (TS f g a b c) m r	

A Pipe for training a model: It consumes mini-batches of samples from upstream and pushes the updated training state downstream.

Pipes API

---

simpleBatchP   # Source

```
:: MonadRandom m
=> [a]                    all available samples
-> Int                    mini-batch size
-> Producer [a] m r
```

A simple `Producer` of mini-batches.

---

cachingBatchP   # Source

```
:: MonadRandom m
=> ([Int] -> m [a])       get samples with specified indices
-> Int                    number of all available samples
-> Int                    mini-batch size
-> Int                    cache size
-> Int                    number of cache reuses
-> Producer [a] m s
```

Function `simpleBatchP` only works when all available samples fit into memory. If this is not the case, `cachingBatchP` can be used instead. It takes an effectful way to get specific samples and then caches some of those samples in memory for a couple of rounds, drawing mini-batches from the cached values.

Pipes API

reportTSP

```
:: Monad m
=> Int                                    report interval
-> (TS f g a b c -> m ())                 report action
-> Pipe (TS f g a b c) (TS f g a b c) m r
```

A Pipe for progress reporting of model training.

consumeTSP

```
:: Monad m
=> (TS f g a b c -> m (Maybe x))   check whether training is finished and what to return in that case
-> Consumer (TS f g a b c) m x
```

A Consumer of training states that decides when training is finished and then returns a value.

Other Features

Other Features

- already implemented

  - fixed-length vectors (used for layers)
  - support for *classification* problems (cross entropy,...)
  - normalization (input whitening)

- work in progress

  - convolutional networks
 - regularization
  - deep learning

Modules

- Data
  - Data.FixedSize fixed-size containers
    - Data.FixedSize.Class class definitions
    - Data.FixedSize.Matrix fixed-size matrices
    - Data.FixedSize.Vector fixed-length vectors
    - Data.FixedSize.Volume fixed-size volumes
  - Data.MyPrelude commonly used standard types and functions
  - Data.Utils various utilities
    - Data.Utils.Analytic "analytic" values
    - Data.Utils.Arrow arrow utilities
    - Data.Utils.Cache caching
    - Data.Utils.List list utilities
    - Data.Utils.Pipes pipe utilities
    - Data.Utils.Random random number utilities
    - Data.Utils.Stack a simple stack monad
    - Data.Utils.Statistics statistical utilities
    - Data.Utils.Traversable utilities for traversables
- Numeric
  - Numeric.Neural neural networks
    - Numeric.Neural.Convolution convolutional layers
    - Numeric.Neural.Layer layer components
    - Numeric.Neural.Model "neural" components and models
    - Numeric.Neural.Normalization normalizing data
    - Numeric.Neural.Pipes a pipes API for models

Examples

Sine Example

- approximate sin(x) on [0, 2π]

- 1 input neuron
- 4 hidden neurons
- 1 output neuron

- accurate to 0.1 after 850 generations
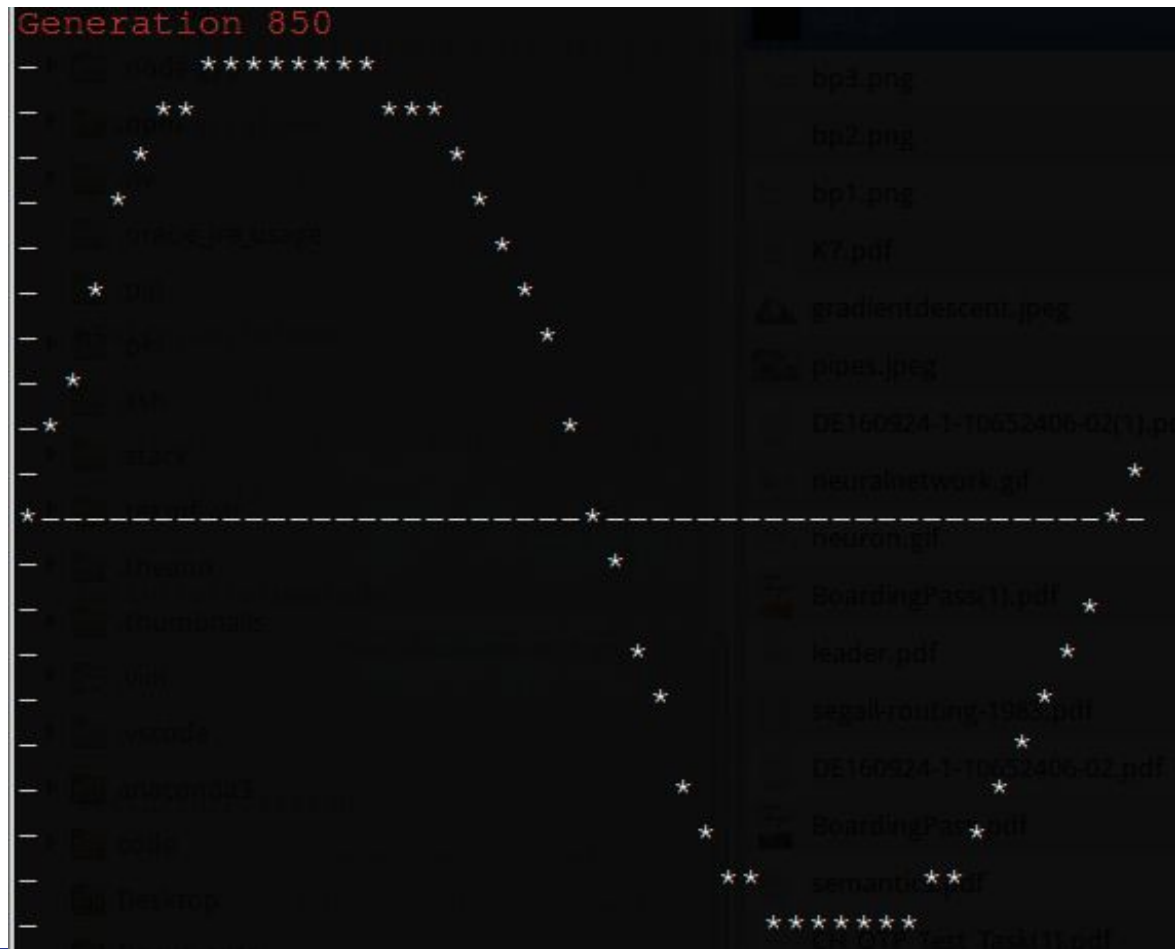
Sine Example

```haskell
main :: IO ()
main = flip evalRandT (mkStdGen 739570) $ do
    let xs = [0, 0.01 .. 2 * pi]
    m <- modelR $ whiten sinModel xs
    runEffect $
            simpleBatchP [(x, sin x) | x <- xs] 10
        >-> descentP m 1 (const 0.5)
        >-> reportTSP 50 report
        >-> consumeTSP check

  where

    sinModel :: StdModel (Vector 1) (Vector 1) Double Double
    sinModel = mkStdModel
        (tanhLayer . (tanhLayer :: Layer 1 4))
        (\x -> Diff $ Identity . sqDiff (pure $ fromDouble x))
        pure
        vhead
```

```haskell
getError ts =
    let m = tsModel ts
    in  maximum [abs (sin x - model m x) | x <- [0, 0.1 .. 2 * pi]]


report ts = liftIO $ do
    ANSI.clearScreen
    ANSI.setSGR [ANSI.SetColor ANSI.Foreground ANSI.Vivid ANSI.Red]
    ANSI.setCursorPosition 0 0
    printf "Generation %d\n" (tsGeneration ts)
    ANSI.setSGR [ANSI.Reset]
    graph (model (tsModel ts)) 0 (2 * pi) 20 50


check ts = return $ if getError ts < 0.1 then Just () else Nothing
```

Other Examples

- sqrt models the similar regression problem of approximating the square root function on the interval [0,4].

- iris solves the famous Iris Flower classification problem.

- MNIST tackles the equally famous MNIST problem of recognizing handwritten digits.

Questions? Comments?