

# 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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on Hackage...

» neural: Neural Networks in native Haskell

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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.



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- 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.

1 branch 5 releases 2 contributors MIT

The library is still very much experimental at this point

Branch: master 92 commits

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Latest commit a6059bb 2 days ago

change the API for much better performance (using "reverse mode" differ...	4 months ago
fixed doctest problem	4 months ago
sin exam...	2 days ago

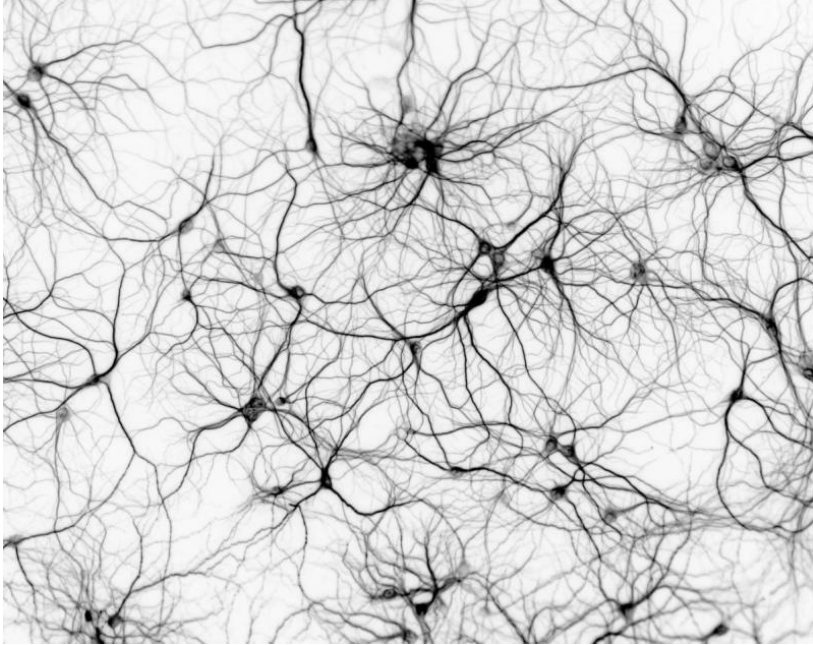
on Hackage...

...and GitHub



# Artificial Neural Networks

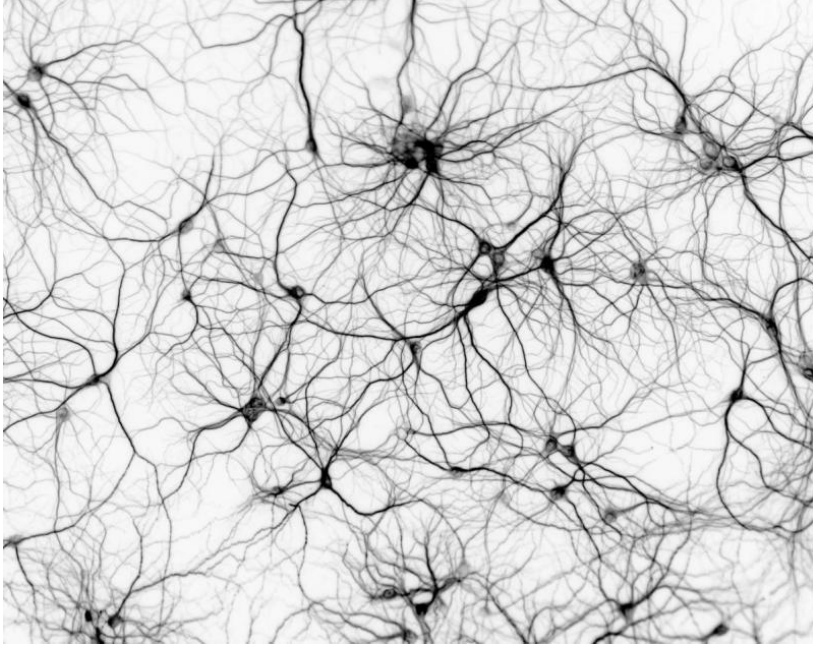
# Artificial Neural Networks



Taking inspiration from biological brains to approach Artificial Intelligence.



# Artificial Neural Networks



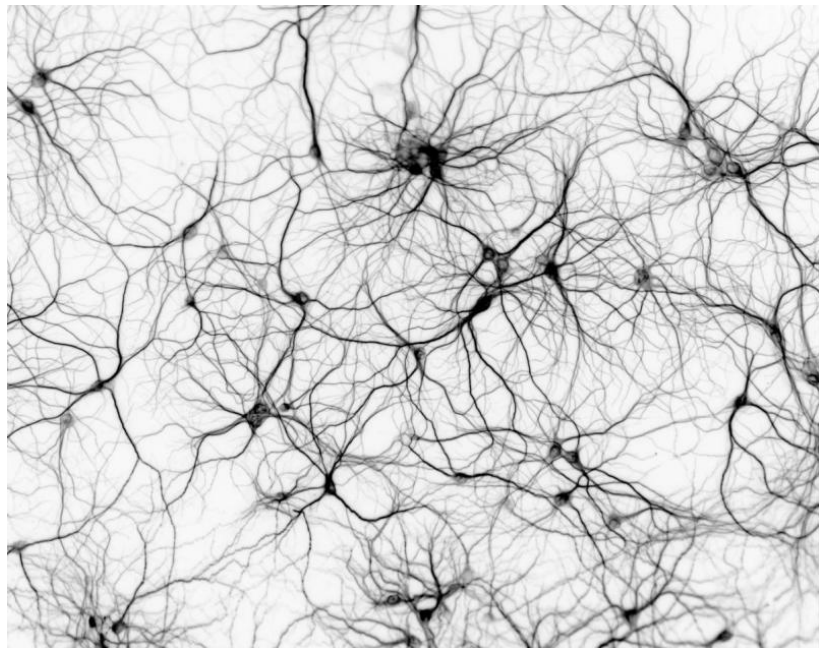
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# Artificial Neural Networks

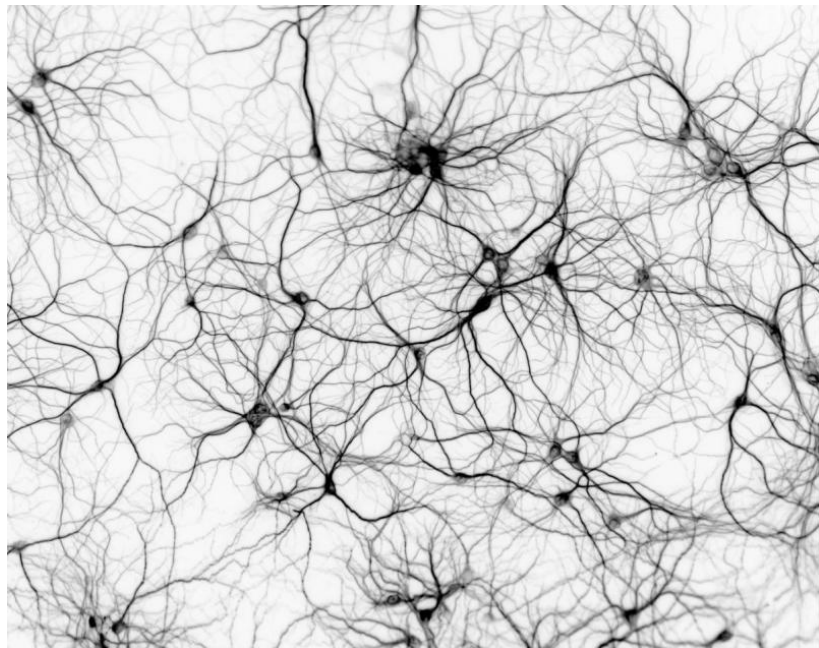


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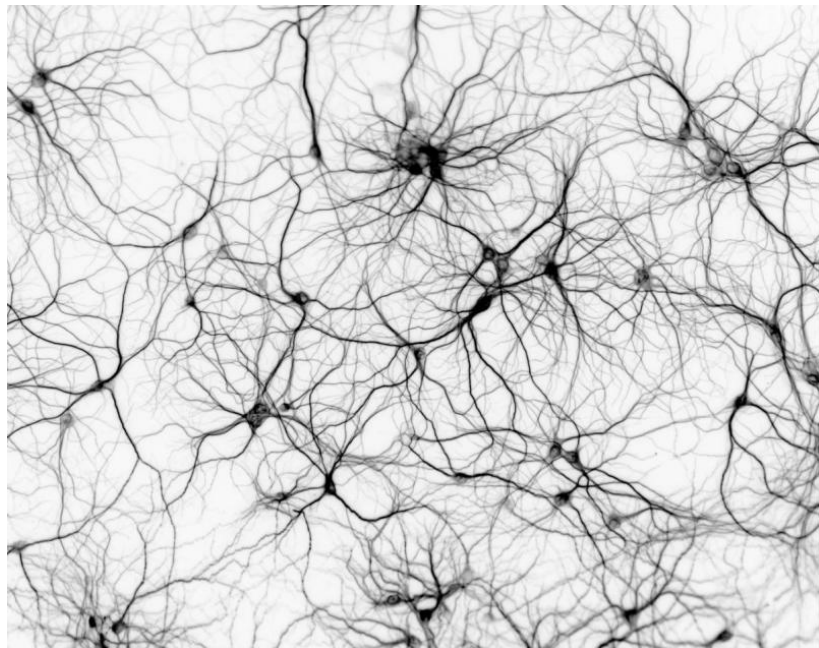


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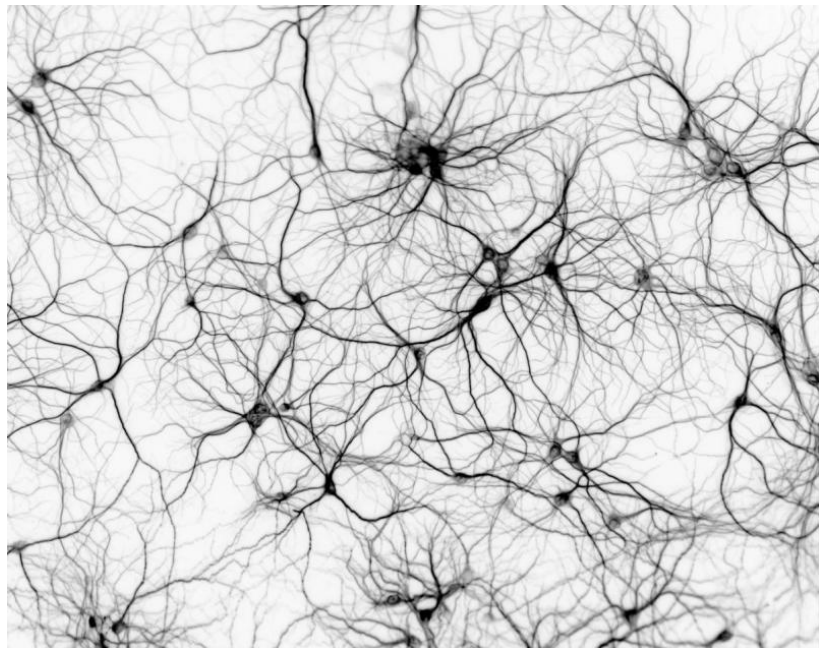


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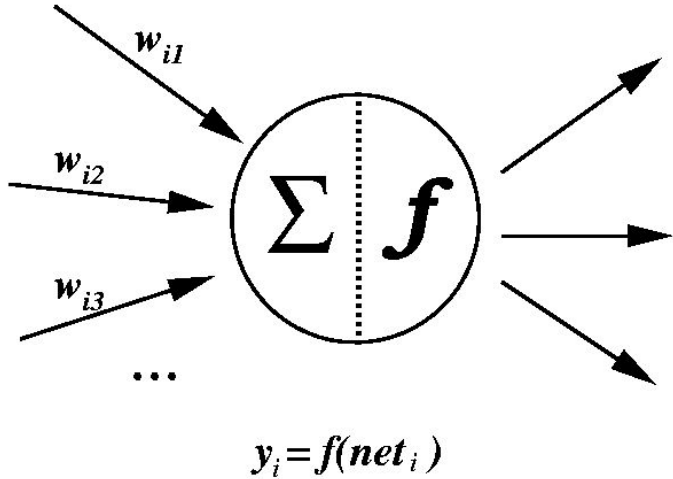


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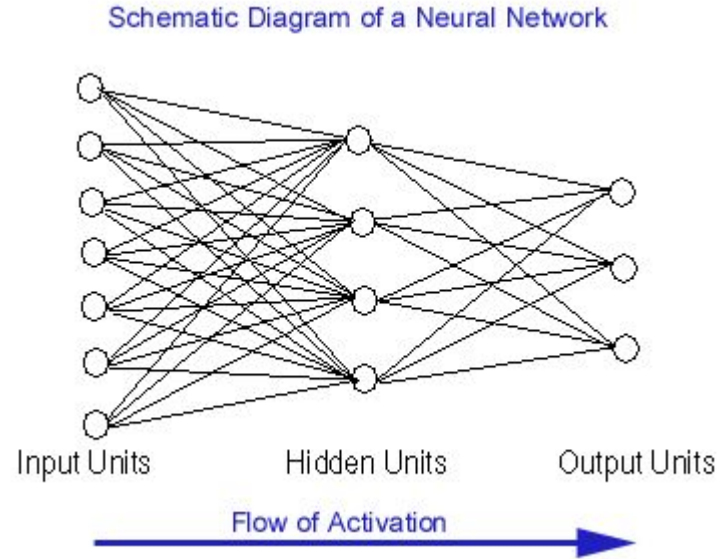
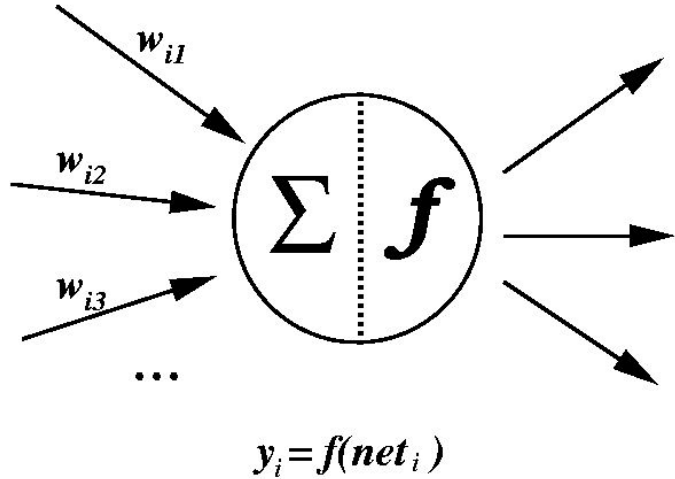


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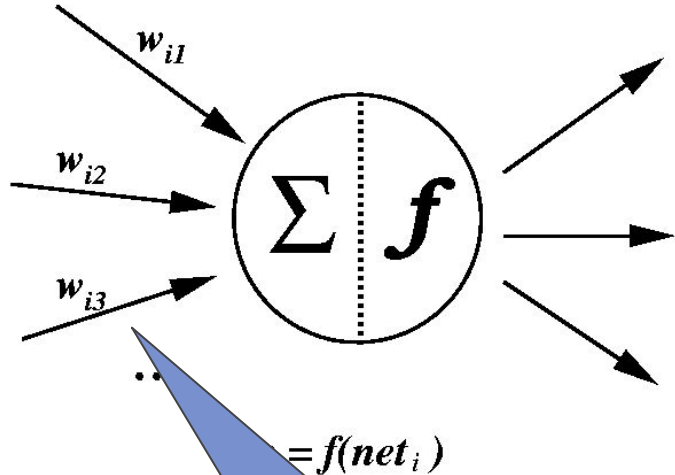




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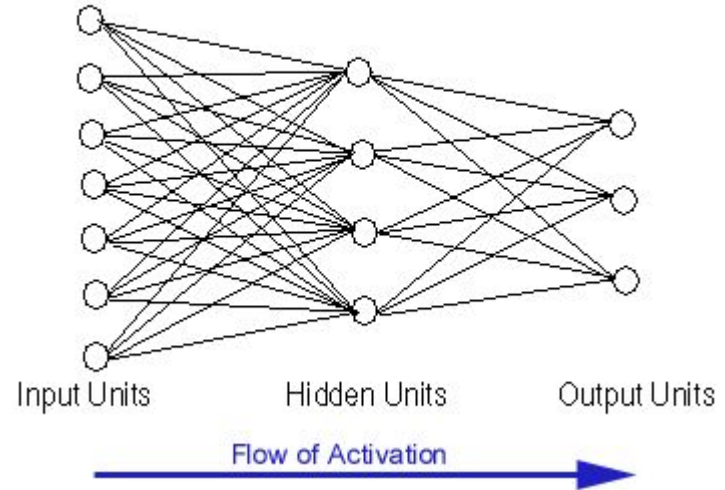


# Artificial Neural Networks



The network learns by adjusting the *weights*

Schematic Diagram of a Neural Network





# Gradient Descent

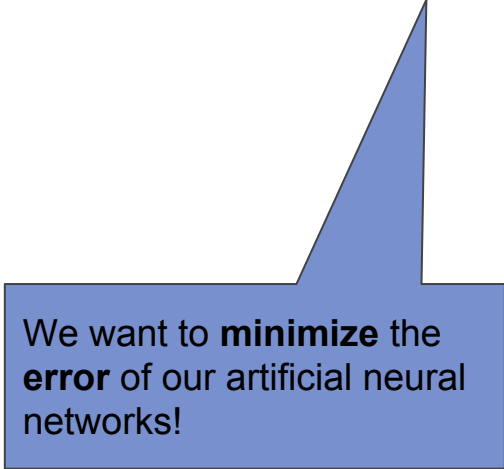
# Gradient Descent

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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All we need is to compute the gradient!



# Backpropagation



# Backpropagation...

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

$$\frac{\partial E_p}{\partial Y_{ji}} = \frac{\partial E_p}{\partial net_{(j+1)1}} \frac{\partial net_{(j+1)1}}{\partial Y_{ji}} + \frac{\partial E_p}{\partial net_{(j+1)2}} \frac{\partial net_{(j+1)2}}{\partial Y_{ji}} + \dots \quad (2.6)$$

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

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

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

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

$$\begin{aligned} \delta_{ji} &= - \sum_{a=1}^{N_{j+1}} [-\delta_{(j+1)a} W_{(j+1)ai}] \frac{\partial Y_{ji}}{\partial net_{ji}} \quad (2.10) \\ &= Y_{ji}(1 - Y_{ji}) \sum_{a=1}^{N_{j+1}} [\delta_{(j+1)a} W_{(j+1)ai}] \quad (2.8) \end{aligned}$$

# ...is just Gradient Descent

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



# Backpropagation

But details change when...



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But details change when...

- A different activation function is used for neurons.



# Backpropagation

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# Backpropagation

But details change when...

- A different activation function is used for neurons.
- A different error function is used.
- A different layout is used.



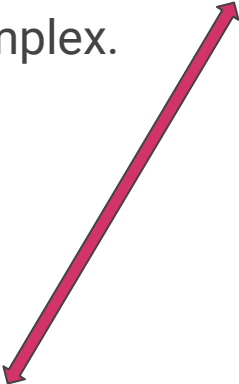
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$$\nabla f = \left( \frac{\partial f}{\partial x_i} \right)_i$$




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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.



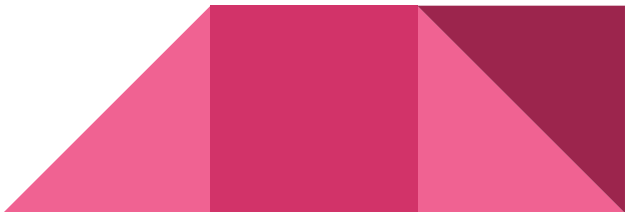
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**Basic Idea:** Manipulate numbers and their derivatives simultaneously (can be done conveniently in Haskell by overloading the numeric type classes).



# Edward Kmett's *ad* Library

```
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.

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

```
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.

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

```
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`.

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

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Arguments of  
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no indices needed!

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```
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Arguments of  
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These types look  
intimidating...

# Neural Wrapper around *ad*

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

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

Minimal complete definition

```
fromDouble
```

Methods

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

Instances

```
+ Analytic Double | # Sou
```

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

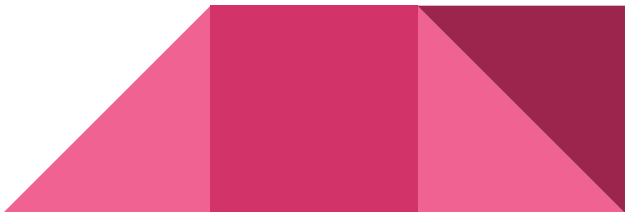
```
+ ArrowChoice (ParamFun s t) | # Source
```

```
+ Profunctor (ParamFun s t) | # Source
```

```
+ ArrowConvolve (ParamFun s t) | # Source
```

```
+ Functor (ParamFun s t a) | # Source
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```
+ Applicative (ParamFun s t a) | # Source
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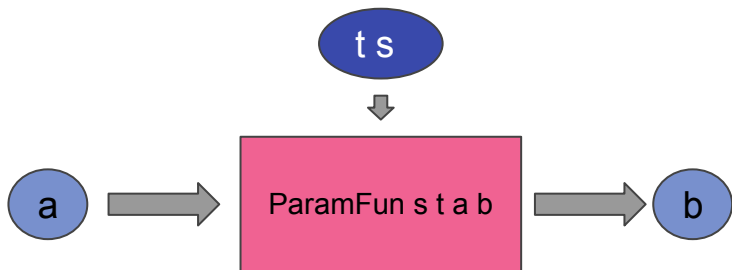
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```



# Components

```
data Component f g
```

```
# Source
```

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

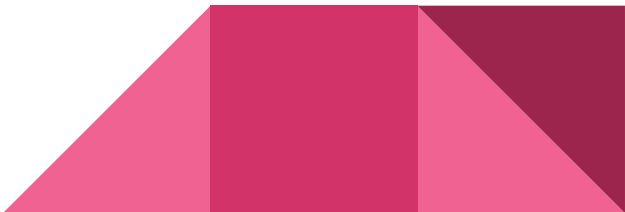
```
initR :: forall m. MonadRandom m => m (t Double)
```

randomly sets the parameters

## Instances

```
⊕ NFData (Component f g) | # Source
```

```
⊕ Category (* -> *) Component | # Source
```



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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
```

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```

```
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 assumption that the error can be computed from the expected output allone.



# Components

## descent

```
:: Foldable h
```

```
=> Model f g a b c
```

```
-> Double
```

```
-> h a
```

```
-> (Double, Model f g a b c)
```

the model whose error should be decreased

the learning rate

a mini-batch of samples

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`.

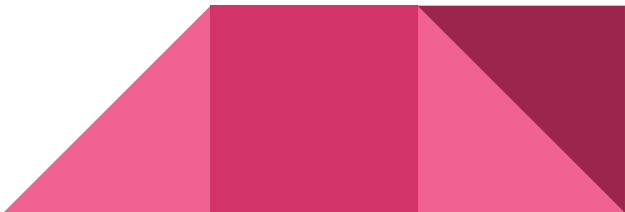
```
linearLayer :: forall i o. (KnownNat i, KnownNat o) => Layer i o
```

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

Modular and flexible components with “built in” gradient descent are nice,  
but not enough: ...



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but not enough:

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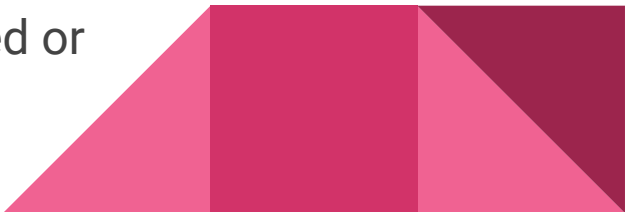
- Training “batches” must be provided - for realistic problems, not all training data will fit into memory.
- We want some progress reporting to see how training is going.





# Pipes API

Modular and flexible components with “built in” gradient descent are nice,  
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.
- 

# Pipes API

This can easily lead to a mess:



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- IO is needed during training to load training data.



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All this tends to produce imperative and non modular code...



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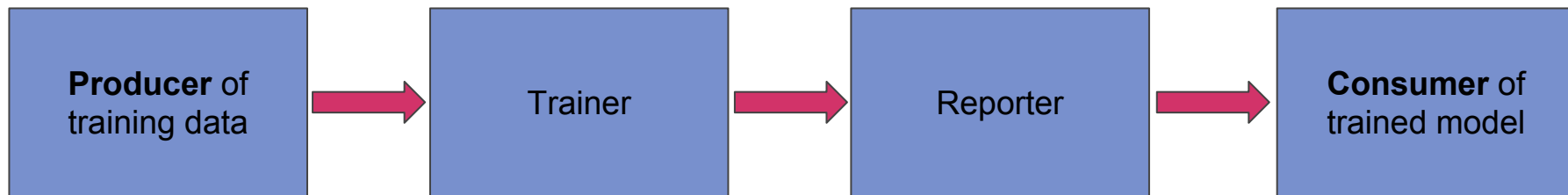
- IO is needed during training to load training data.
- Progress reporting has to be mixed with training code.
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All this tends to produce imperative and non modular code...

**Pipes to the rescue!**



# Pipes API





# Pipes API

data TS f g a b c

# Source

Extensions

BangPatterns

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

# Source

:: (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

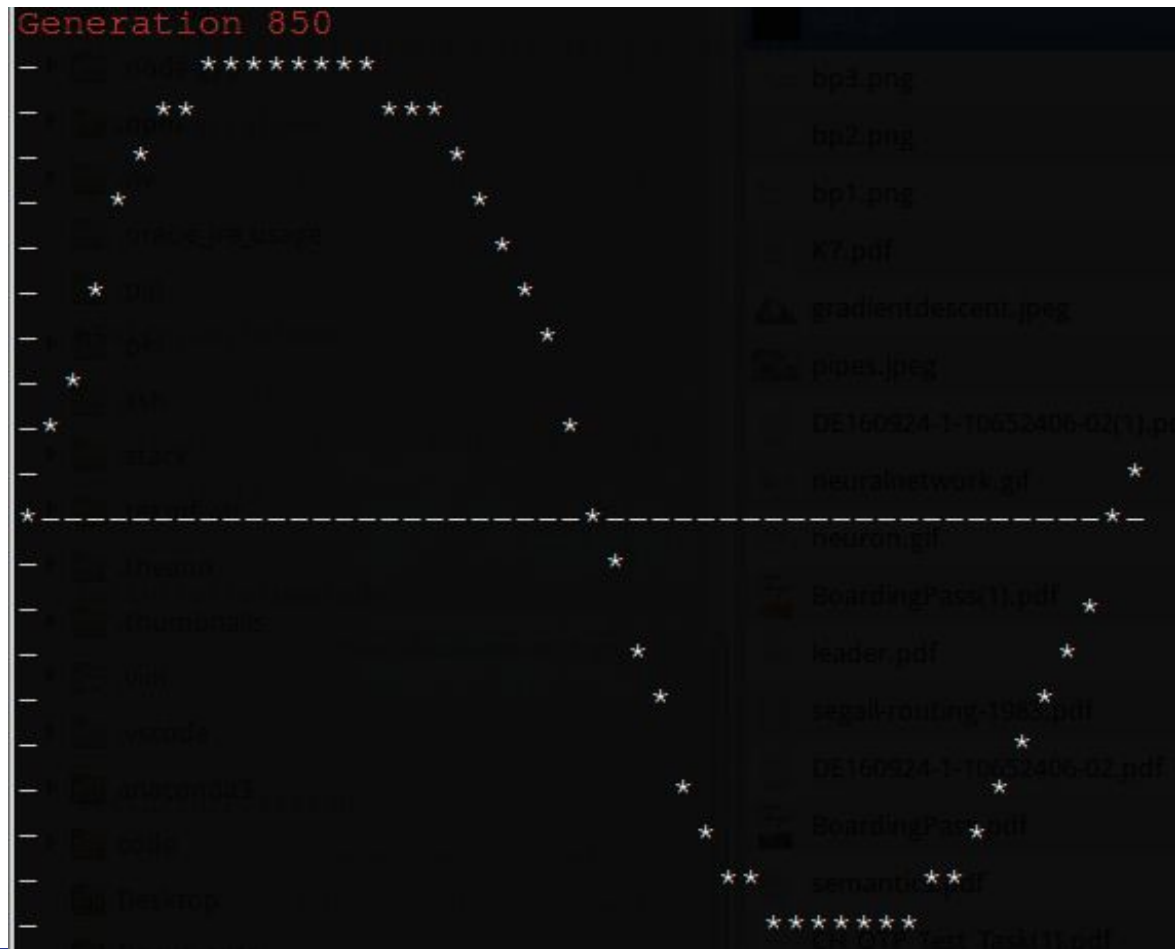
## Modules

- ▢ 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.Utls` various utilities
    - `Data.Utls.Analytic` "analytic" values
    - `Data.Utls.Arrow` arrow utilities
    - `Data.Utls.Cache` caching
    - `Data.Utls.List` list utilities
    - `Data.Utls.Pipes` pipe utilities
    - `Data.Utls.Random` random number utilities
    - `Data.Utls.Stack` a simple stack monad
    - `Data.Utls.Statistics` statistical utilities
    - `Data.Utls.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  $[0, 2\pi]$
- 1 input neuron
- 4 hidden neurons
- 1 output neuron
- accurate to 0.1 after 850 generations



# Sine Example

```
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
```

```
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.



A microscopic image of neurons, showing a central cell body with multiple branching processes. The image is overlaid with a blue geometric pattern in the top right corner, consisting of several triangles of different shades of blue. The text "Questions? Comments?" is centered in the image.

Questions? Comments?