Extensible Neural Networks with Backprop

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This write-up is a follow-up to the *MNIST* tutorial (rendered[1] here, and literate haskell[2] here). This write-up itself is available as a literate haskell file[3], and also rendered as a pdf[4].

The packages involved are:

- deepseq
- hmatrix
- lens
- mnist-idx
- mwc-random
- one-liner-instances
- singletons
- split
- vector

```
{-# LANGUAGE BangPatterns        #-}
{-# LANGUAGE DataKinds           #-}
{-# LANGUAGE DeriveGeneric       #-}
{-# LANGUAGE FlexibleContexts    #-}
{-# LANGUAGE GADTs               #-}
{-# LANGUAGE InstanceSigs        #-}
{-# LANGUAGE LambdaCase          #-}
{-# LANGUAGE LambdaCase          #-}
{-# LANGUAGE RankNTypes          #-}
{-# LANGUAGE ScopedTypeVariables #-}
{-# LANGUAGE TemplateHaskell     #-}
{-# LANGUAGE TypeApplications    #-}
{-# LANGUAGE TypeInType          #-}
{-# LANGUAGE TypeOperators       #-}
{-# LANGUAGE ViewPatterns        #-}
{-# OPTIONS_GHC -fno-warn-orphans #-}

import           Control.DeepSeq
import           Control.Exception
import           Control.Lens hiding            ((<.>))
import           Control.Monad
import           Control.Monad.IO.Class
import           Control.Monad.Primitive
import           Control.Monad.Trans.Maybe
import           Control.Monad.Trans.State
import           Data.Bitraversable
```

[1] https://github.com/mstksg/backprop/blob/master/renders/backprop-mnist.pdf
[2] https://github.com/mstksg/backprop/blob/master/samples/backprop-mnist.lhs
[3] https://github.com/mstksg/backprop/blob/master/samples/extensible-neural.lhs
[4] https://github.com/mstksg/backprop/blob/master/renders/extensible-neural.pdf

```haskell
import           Data.Foldable
import           Data.IDX
import           Data.Kind
import           Data.List.Split
import           Data.Singletons
import           Data.Singletons.Prelude
import           Data.Singletons.TypeLits
import           Data.Time.Clock
import           Data.Traversable
import           Data.Tuple
import           GHC.Generics                     (Generic)
import           Numeric.Backprop
import           Numeric.LinearAlgebra.Static
import           Numeric.OneLiner
import           Text.Printf
import qualified Data.Vector                      as V
import qualified Data.Vector.Generic              as VG
import qualified Data.Vector.Unboxed              as VU
import qualified Numeric.LinearAlgebra            as HM
import qualified System.Random.MWC                as MWC
import qualified System.Random.MWC.Distributions as MWC
```

Introduction

The *backprop*[5] library lets us manipulate our values in a natural way. We write the function to compute our result, and the library then automatically finds the *gradient* of that function, which we can use for gradient descent.

In the last post, we looked at using a fixed-structure neural network. However, in this blog series[6], I discuss a system of extensible neural networks that can be chained and composed.

One issue, however, in naively translating the implementations, is that we normally run the network by pattern matching on each layer. However, we cannot directly pattern match on `BVar`s.

We *could* get around it by being smart with prisms and `^^?`, to extract a "Maybe BVar". However, we can do better! This is because the *shape* of a `Net i hs o` is known already at compile-time, so there is no need for runtime checks like prisms and `^^?`.

Instead, we can just directly use lenses, since we know *exactly* what constructor will be present! We can use singletons to determine which constructor is present, and so always just directly use lenses without any runtime nondeterminism.

Types

First, our types:

```haskell
data Layer i o =
    Layer { _lWeights :: !(L o i)
          , _lBiases  :: !(R o)
          }
```

[5] http://hackage.haskell.org/package/backprop
[6] https://blog.jle.im/entries/series/+practical-dependent-types-in-haskell.html

```haskell
  deriving (Show, Generic)

instance NFData (Layer i o)
makeLenses ''Layer

data Net :: Nat -> [Nat] -> Nat -> Type where
    NO   :: !(Layer i o) -> Net i '[] o
    (:~) :: !(Layer i h) -> !(Net h hs o) -> Net i (h ': hs) o
```

Unfortunately, we can't automatically generate lenses for GADTs, so we have to make them by hand.[^poly]

with type safety via paraemtric polymorphism.

```haskell
_NO :: Lens (Net i '[] o) (Net i' '[] o')
            (Layer i o  ) (Layer i' o'  )
_NO f (NO l) = NO <$> f l

_NIL :: Lens (Net i (h ': hs) o) (Net i' (h ': hs) o)
             (Layer i h         ) (Layer i' h         )
_NIL f (l :~ n) = (:~ n) <$> f l

_NIN :: Lens (Net i (h ': hs) o) (Net i (h ': hs') o')
             (Net h hs        o) (Net h hs'        o')
_NIN f (l :~ n) = (l :~) <$> f n
```

You can read `_NO` as:

```haskell
_NO :: Lens' (Net i '[] o) (Layer i o)
```

A lens into a single-layer network, and

```haskell
_NIL :: Lens' (Net i (h ': hs) o) (Layer i h )
_NIN :: Lens' (Net i (h ': hs) o) (Net h hs o)
```

Lenses into a multiple-layer network, getting the first layer and the tail of the network.

If we pattern match on `Sing hs`, we can always determine exactly which lenses we can use, and so never fumble around with prisms or nondeterminism.

Running the network

Here's the meat of process, then: specifying how to run the network. We re-use our `BVar`-based combinators defined in the last write-up:

```haskell
runLayer
    :: (KnownNat i, KnownNat o, Reifies s W)
    => BVar s (Layer i o)
    -> BVar s (R i)
    -> BVar s (R o)
runLayer l x = (l ^^. lWeights) #>! x + (l ^^. lBiases)
{-# INLINE runLayer #-}
```

For `runNetwork`, we pattern match on `hs` using singletons, so we always know exactly what type of network we have:

```haskell
runNetwork
    :: (KnownNat i, KnownNat o, Reifies s W)
```

```haskell
    => BVar s (Net i hs o)
    -> Sing hs
    -> BVar s (R i)
    -> BVar s (R o)
runNetwork n = \case
    SNil          -> softMax . runLayer (n ^^. _NO)
    SCons SNat hs -> withSingI hs (runNetwork (n ^^. _NIN) hs)
                   . logistic
                   . runLayer (n ^^. _NIL)
{-# INLINE runNetwork #-}
```

The rest of it is the same as before.

```haskell
netErr
    :: (KnownNat i, KnownNat o, SingI hs, Reifies s W)
    => R i
    -> R o
    -> BVar s (Net i hs o)
    -> BVar s Double
netErr x targ n = crossEntropy targ (runNetwork n sing (constVar x))
{-# INLINE netErr #-}

trainStep
    :: forall i hs o. (KnownNat i, KnownNat o, SingI hs)
    => Double             -- ^ learning rate
    -> R i                -- ^ input
    -> R o                -- ^ target
    -> Net i hs o         -- ^ initial network
    -> Net i hs o
trainStep r !x !targ !n = n - realToFrac r * gradBP (netErr x targ) n
{-# INLINE trainStep #-}

trainList
    :: (KnownNat i, SingI hs, KnownNat o)
    => Double             -- ^ learning rate
    -> [(R i, R o)]       -- ^ input and target pairs
    -> Net i hs o         -- ^ initial network
    -> Net i hs o
trainList r = flip $ foldl' (\n (x,y) -> trainStep r x y n)
{-# INLINE trainList #-}

testNet
    :: forall i hs o. (KnownNat i, KnownNat o, SingI hs)
    => [(R i, R o)]
    -> Net i hs o
    -> Double
testNet xs n = sum (map (uncurry test) xs) / fromIntegral (length xs)
  where
    test :: R i -> R o -> Double          -- test if the max index is correct
    test x (extract->t)
        | HM.maxIndex t == HM.maxIndex (extract r)  = 1
        | otherwise                                 = 0
      where
        r :: R o
```

```
        r = evalBP (\n' -> runNetwork n' sing (constVar x)) n
```

And that's it!

Running

Everything here is the same as before, except now we can dynamically pick the network size. Here we pick `'[300,100]` for the hidden layer sizes.

```
main :: IO ()
main = MWC.withSystemRandom $ \g -> do
    Just train <- loadMNIST "data/train-images-idx3-ubyte" "data/train-labels-idx1-ubyte"
    Just test  <- loadMNIST "data/t10k-images-idx3-ubyte"  "data/t10k-labels-idx1-ubyte"
    putStrLn "Loaded data."
    net0 <- MWC.uniformR @(Net 784 '[300,100] 10) (-0.5, 0.5) g
    flip evalStateT net0 . forM_ [1..] $ \e -> do
      train' <- liftIO . fmap V.toList $ MWC.uniformShuffle (V.fromList train) g
      liftIO $ printf "[Epoch %d]\n" (e :: Int)

      forM_ ([1..] `zip` chunksOf batch train') $ \(b, chnk) -> StateT $ \n0 -> do
        printf "(Batch %d)\n" (b :: Int)

        t0 <- getCurrentTime
        n' <- evaluate . force $ trainList rate chnk n0
        t1 <- getCurrentTime
        printf "Trained on %d points in %s.\n" batch (show (t1 `diffUTCTime` t0))

        let trainScore = testNet chnk n'
            testScore  = testNet test n'
        printf "Training error:   %.2f%%\n" ((1 - trainScore) * 100)
        printf "Validation error: %.2f%%\n" ((1 - testScore ) * 100)

        return ((), n')
  where
    rate  = 0.02
    batch = 5000
```

Looking Forward

One common thing people might do is want to be able to mix different types of layers. This could also be easily encoded as different constructors in `Layer`, and so `runLayer` will now be different depending on what constructor is present.

In this case, we can either:

1. Have a different indexed type for layers, so that we can always know exactly what layer is involved, so we don't have to runtime pattern match:

   ```
   data LayerType = FullyConnected | Convolutional

   data Layer :: LayerType -> Nat -> Nat -> Type where
   ```

```
    LayerFC :: .... -> Layer 'FullyConnected i o
    LayerC  :: .... -> Layer 'Convolutional  i o
```

We would then have `runLayer` take `Sing (t :: LayerType)`, so we can again use `^^.` and directly pattern match.

2. Use a typeclass-based approach, so users can add their own layer types. In this situation, layer types would all be different types, and running them would be a typeclass method that would give our `BVar s (Layer i o) -> BVar s (R i) -> BVar s (R o)` operation as a typeclass method.

```
class Layer (l :: Nat -> Nat -> Type) where
    runLayer
        :: forall s. Reifies s W
        => BVar s (l i o)
        -> BVar s (R i)
        -> BVar s (R o)
```

In all cases, it shouldn't be much more cognitive overhead to use *backprop* to build your neural network framework!

And, remember that `evalBP` (directly running the function) introduces virtually zero overhead, so if you only provided `BVar` functions, you could easily get the original non-`BVar` functions with `evalBP` without any loss.

What now?

Ready to start? Check out the docs for the Numeric.Backprop[7] module for the full technical specs, and find more examples and updates at the github repo[8]!

Internals

That's it for the post! Now for the internal plumbing :)

```
loadMNIST
    :: FilePath
    -> FilePath
    -> IO (Maybe [(R 784, R 10)])
loadMNIST fpI fpL = runMaybeT $ do
    i <- MaybeT          $ decodeIDXFile       fpI
    l <- MaybeT          $ decodeIDXLabelsFile fpL
    d <- MaybeT . return $ labeledIntData l i
    r <- MaybeT . return $ for d (bitraverse mkImage mkLabel . swap)
    liftIO . evaluate $ force r
  where
    mkImage :: VU.Vector Int -> Maybe (R 784)
    mkImage = create . VG.convert . VG.map (\i -> fromIntegral i / 255)
    mkLabel :: Int -> Maybe (R 10)
    mkLabel n = create $ HM.build 10 (\i -> if round i == n then 1 else 0)
```

[7] http://hackage.haskell.org/package/backprop/docs/Numeric-Backprop.html
[8] https://github.com/mstksg/backprop

HMatrix Operations

```haskell
infixr 8 #>!
(#>!)
    :: (KnownNat m, KnownNat n, Reifies s W)
    => BVar s (L m n)
    -> BVar s (R n)
    -> BVar s (R m)
(#>!) = liftOp2 . op2 $ \m v ->
  ( m #> v, \g -> (g `outer` v, tr m #> g) )

infixr 8 <.>!
(<.>!)
    :: (KnownNat n, Reifies s W)
    => BVar s (R n)
    -> BVar s (R n)
    -> BVar s Double
(<.>!) = liftOp2 . op2 $ \x y ->
  ( x <.> y, \g -> (konst g * y, x * konst g)
  )

konst'
    :: (KnownNat n, Reifies s W)
    => BVar s Double
    -> BVar s (R n)
konst' = liftOp1 . op1 $ \c -> (konst c, HM.sumElements . extract)

sumElements'
    :: (KnownNat n, Reifies s W)
    => BVar s (R n)
    -> BVar s Double
sumElements' = liftOp1 . op1 $ \x -> (HM.sumElements (extract x), konst)

softMax :: (KnownNat n, Reifies s W) => BVar s (R n) -> BVar s (R n)
softMax x = konst' (1 / sumElements' expx) * expx
  where
    expx = exp x
{-# INLINE softMax #-}

crossEntropy
    :: (KnownNat n, Reifies s W)
    => R n
    -> BVar s (R n)
    -> BVar s Double
crossEntropy targ res = -(log res <.>! constVar targ)
{-# INLINE crossEntropy #-}

logistic :: Floating a => a -> a
logistic x = 1 / (1 + exp (-x))
{-# INLINE logistic #-}
```

Instances

```haskell
instance (KnownNat i, KnownNat o) => Num (Layer i o) where
    (+)         = gPlus
    (-)         = gMinus
    (*)         = gTimes
    negate      = gNegate
    abs         = gAbs
    signum      = gSignum
    fromInteger = gFromInteger

instance (KnownNat i, KnownNat o) => Fractional (Layer i o) where
    (/)          = gDivide
    recip        = gRecip
    fromRational = gFromRational


liftNet0
    :: forall i hs o. (KnownNat i, KnownNat o)
    => (forall m n. (KnownNat m, KnownNat n) => Layer m n)
    -> Sing hs
    -> Net i hs o
liftNet0 x = go
  where
    go :: forall w ws. KnownNat w => Sing ws -> Net w ws o
    go = \case
      SNil          -> NO x
      SCons SNat hs -> x :~ go hs

liftNet1
    :: forall i hs o. (KnownNat i, KnownNat o)
    => (forall m n. (KnownNat m, KnownNat n)
          => Layer m n
          -> Layer m n
       )
    -> Sing hs
    -> Net i hs o
    -> Net i hs o
liftNet1 f = go
  where
    go  :: forall w ws. KnownNat w
        => Sing ws
        -> Net w ws o
        -> Net w ws o
    go = \case
      SNil          -> \case
        NO x -> NO (f x)
      SCons SNat hs -> \case
        x :~ xs -> f x :~ go hs xs

liftNet2
    :: forall i hs o. (KnownNat i, KnownNat o)
    => (forall m n. (KnownNat m, KnownNat n)
```

```haskell
          => Layer m n
          -> Layer m n
          -> Layer m n
       )
    -> Sing hs
    -> Net i hs o
    -> Net i hs o
    -> Net i hs o
liftNet2 f = go
  where
    go  :: forall w ws. KnownNat w
        => Sing ws
        -> Net w ws o
        -> Net w ws o
        -> Net w ws o
    go = \case
      SNil          -> \case
        NO x -> \case
          NO y -> NO (f x y)
      SCons SNat hs -> \case
        x :~ xs -> \case
          y :~ ys -> f x y :~ go hs xs ys

instance ( KnownNat i
         , KnownNat o
         , SingI hs
         )
      => Num (Net i hs o) where
    (+)           = liftNet2 (+) sing
    (-)           = liftNet2 (-) sing
    (*)           = liftNet2 (*) sing
    negate        = liftNet1 negate sing
    abs           = liftNet1 abs sing
    signum        = liftNet1 signum sing
    fromInteger x = liftNet0 (fromInteger x) sing

instance ( KnownNat i
         , KnownNat o
         , SingI hs
         )
      => Fractional (Net i hs o) where
    (/)            = liftNet2 (/) sing
    recip          = liftNet1 negate sing
    fromRational x = liftNet0 (fromRational x) sing

instance KnownNat n => MWC.Variate (R n) where
    uniform g = randomVector <$> MWC.uniform g <*> pure Uniform
    uniformR (l, h) g = (\x -> x * (h - l) + l) <$> MWC.uniform g

instance (KnownNat m, KnownNat n) => MWC.Variate (L m n) where
    uniform g = uniformSample <$> MWC.uniform g <*> pure 0 <*> pure 1
    uniformR (l, h) g = (\x -> x * (h - l) + l) <$> MWC.uniform g
```

```haskell
instance (KnownNat i, KnownNat o) => MWC.Variate (Layer i o) where
    uniform g = Layer <$> MWC.uniform g <*> MWC.uniform g
    uniformR (l, h) g = (\x -> x * (h - l) + l) <$> MWC.uniform g

instance ( KnownNat i
         , KnownNat o
         , SingI hs
         )
      => MWC.Variate (Net i hs o) where
    uniform :: forall m. PrimMonad m => MWC.Gen (PrimState m) -> m (Net i hs o)
    uniform g = go sing
      where
        go :: forall w ws. KnownNat w => Sing ws -> m (Net w ws o)
        go = \case
          SNil          -> NO <$> MWC.uniform g
          SCons SNat hs -> (:~) <$> MWC.uniform g <*> go hs
    uniformR (l, h) g = (\x -> x * (h - l) + l) <$> MWC.uniform g

instance NFData (Net i hs o) where
    rnf = \case
      NO l    -> rnf l
      x :~ xs -> rnf x `seq` rnf xs
```