Multi-Layer NN

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Generate Data

For now, having 3 inputs and combining them to create y, with a random error term. Would like to tweak the setup eventually.

```r
## create data:
m <- 1000
n_1_manual <- 3
n_L_manual <- 1

# initialize Xs
X <- data.frame(X1 = runif(n = m, min = -10, max = 10),
                X2 = rnorm(n = m, mean = 0, sd = 10),
                X3 = rexp(n = m, rate = 1)) %>%
  as.matrix(nrow = m,
            ncol = n_1_manual)

# get response
Y <- X[, 1] + 10 * sin(X[, 2])^2 + 10 * X[, 3] + rnorm(n = 1000)

# fix dims according to NN specs
X <- t(X)
Y <- t(Y)
```

Functions

Link Functions

```r
## Specify Link Functions & Derivatives
get_link <- function(type = "sigmoid") {

  if (type == "identity") {
    # identity
    g <- function(x) {x}

  } else if (type == "sigmoid") {
    # sigmoid
    g <- function(x) {1 / (1 + exp(-x))}

  } else if (type == "relu") {
```

```r
    # ReLU
    g <- function(x) {x * as.numeric(x > 0)}

  } else (return(NULL))

  return(g)

}

get_link_prime <- function(type = "sigmoid") {

  if (type == "identity") {
    # identity [FIX]
    g_prime <- function(x) {
      ## there's probably a better way to do this
      b <- x / x
      b[is.nan(x/x)] <- 1
      return(b)
    }

  } else if (type == "sigmoid") {
    # sigmoid
    g_prime <- function(x) {exp(-x) / (1 + exp(-x))^2}

  } else if (type == "relu") {
    # ReLU
    g_prime <- function(x) {as.numeric(x > 0)}

  } else (return(NULL))

  return(g_prime)

}
```

Loss Functions

```r
## Specify Loss Functions & Derivatives
get_loss_function <- function(type = "squared_error") {

  if (type == "squared_error") {

    loss <- function(y_hat, y) {sum((y_hat - y)^2)}

  } else if (type == "cross_entropy") {

    loss <- function(y_hat, y) {sum(y * log(y_hat))}

  } else (return(NULL))

  return(loss)

}
```

```r
get_loss_prime <- function(type = "squared_error") {

  if (type == "squared_error") {

    loss_prime <- function(y_hat, y) {sum(2 * (y_hat - y))}

  } else if (type == "cross_entropy") {

    loss_prime <- function(y_hat, y) {999}

  } else (return(NULL))

  return(loss_prime)

}
```

Misc Helpers

```r
## creates a list of n empty lists
create_lists <- function(n) {
  out <- list()

  for (i in 1:n) {
    out[[i]] <- list()
  }

  return(out)
}

## friendlier diag() function
diag_D <- function(x) {

  if (length(x) == 1) {
        out <- x
      } else {
        out <- diag(as.numeric(x))
      }

  return(out)
}

fetch_layer_sizes <- function(X,
                              Y,
                              hidden_layer_sizes) {

  return(c(nrow(X), hidden_layers, nrow(Y)))

}
```

```r
initialize_NN <- function(layer_sizes,
                          activation_function = "sigmoid",
```

```
                          last_activation_function = "identity",
                          lower_bound = 0,
                          upper_bound = 1) {

  n <- layer_sizes

  ## initialize parameter matrices
  W <- list()
  b <- list()

  ## could vectorize w/ mapply()
  for (l in 2:length(n)) {

    W[[l]] <- matrix(data = runif(n = n[l - 1] * n[l],
                                  min = lower_bound,
                                  max = upper_bound),
                     nrow = n[l],
                     ncol = n[l - 1])

    b[[l]] <- matrix(data = runif(n = n[l],
                                  min = lower_bound,
                                  max = upper_bound),
                     nrow = n[l],
                     ncol = 1)

  }

  ## return
  return(list(W = W,
              b = b,
              activation_function = activation_function,
              last_activation_function = last_activation_function))
}
```

Forward Propagation

```
NN_output <- function(X,
                      NN_obj) {

  L <- length(NN_obj$W)
  ## if X is one obs, input will be a vector so dim will be null
  m <- ifelse(is.null(ncol(X)),
              1,
              ncol(X))

  g <- get_link(NN_obj$activation_function)
  g_last <- get_link(NN_obj$last_activation_function)

  a <- list()

  a[[1]] <- X
```

```
  for (l in 2:(L - 1)) {
    a[[l]] <- g(NN_obj$W[[l]] %*% a[[l - 1]] + matrix(data = rep(x = NN_obj$b[[l]],
                                                                  times = m),
                                                       ncol = m))
  }

  a[[L]] <- g_last(NN_obj$W[[L]] %*% a[[L - 1]] + matrix(data = rep(x = NN_obj$b[[L]],
                                                                  times = m),
                                                       ncol = m))

  return(a[[L]])

}
```

Gradient Descent Iteration

```
GD_iter <- function(NN_obj,
                    X,
                    Y,
                    rho = 1,
                    verbose = FALSE,
                    very_verbose = FALSE) {

  L <- length(NN_obj$W)
  ## if X is one obs, input will be a vector so dim will be null
  m <- ifelse(is.null(ncol(X)),
              1,
              ncol(X))

  ## get links
  g <- get_link(NN_obj$activation_function)
  g_prime <- get_link_prime(NN_obj$activation_function)
  g_last <- get_link(NN_obj$last_activation_function)
  g_last_prime <- get_link_prime(NN_obj$last_activation_function)

  z <- create_lists(L)
  a <- create_lists(L)
  D <- create_lists(L)
  delta <- create_lists(L)
  del_W <- create_lists(L)
  del_b <- create_lists(L)

  ## gradient descent
  for (i in 1:m) {

    ## forward
    a[[1]][[i]] <- X[, i]

    for (l in 2:(L - 1)) {
      z[[l]][[i]] <- NN_obj$W[[l]] %*% a[[l - 1]][[i]] + NN_obj$b[[l]]
      a[[l]][[i]] <- g(z[[l]][[i]])
```

```r
    D[[l]][[i]] <- diag_D(g_prime(z[[l]][[i]]))

    if (very_verbose == TRUE) {print(paste0("Forward: obs ", i, " - layer ", l))}
  }

  ## last layer
  z[[L]][[i]] <- NN_obj$W[[L]] %*% a[[L - 1]][[i]] + NN_obj$b[[L]]
  a[[L]][[i]] <- g_last(z[[L]][[i]])
  D[[L]][[i]] <- diag_D(g_last_prime(z[[L]][[i]]))

  ## backward
  # eventually fix to match with loss function
  delta[[L]][[i]] <- D[[L]][[i]] %*% (a[[L]][[i]] - Y[, i])

  for (l in (L - 1):2) {
    delta[[l]][[i]] <- D[[l]][[i]] %*% t(NN_obj$W[[l + 1]]) %*% delta[[l + 1]][[i]]
    if (very_verbose == TRUE) {print(paste0("Backward: obs ", i, " - layer ", l))}
  }

  for (l in 2:L) {
    del_W[[l]][[i]] <- delta[[l]][[i]] %*% t(a[[l - 1]][[i]])
    del_b[[l]][[i]] <- delta[[l]][[i]]
    if (very_verbose == TRUE) {print(paste0("del: obs ", i, " - layer ", l))}
  }

  if ((verbose == TRUE) & (i %% 100 == 0)) {print(paste("obs", i, "/", m))}

}

## update parameters

# get averages
## del_W is a list where each element represents a layer
## in each layer, there's a list representing the layer's result for that obs
## here we collapse the results by taking the sum of our gradients
del_W_all <- lapply(X = del_W,
                    FUN = Reduce,
                    f = "+") %>%
  lapply(X = .,
         FUN = function(x) x / m)

del_b_all <- lapply(X = del_b,
                    FUN = Reduce,
                    f = "+") %>%
  lapply(X = .,
         FUN = function(x) x / m)

# apply gradient
W_out <- mapply(FUN = function(A, del_A) {A - rho * del_A},
                A = NN_obj$W,
                del_A = del_W_all)

b_out <- mapply(FUN = function(A, del_A) {A - rho * del_A},
```

```
                  A = NN_obj$b,
                  del_A = del_b_all)

  ## return a new NN object
  return(list(W = W_out,
              b = b_out,
              activation_function = NN_obj$activation_function,
              last_activation_function = NN_obj$last_activation_function))
}
```

Perform Gradient Descent

```
GD_perform <- function(X,
                       Y,
                       init_NN_obj,
                       rho = 0.01,
                       loss_function = "squared_error",
                       threshold = 1,
                       max_iter = 100,
                       print_descent = FALSE) {

  ## setup
  done_decreasing <- FALSE

  objective_function <- get_loss_function(type = loss_function)

  iteration_outputs <- list()
  output_objectives <- numeric()

  iteration_input <- init_NN_obj

  iter <- 1

  initial_objective <- objective_function(y = Y,
                                          y_hat = NN_output(X = X,
                                                            NN_obj = init_NN_obj))

  if (print_descent == TRUE) {
    print(paste0("iter: ", 0, "; obj: ", round(initial_objective, 1)))
  }

  while ((!done_decreasing) & (iter < max_iter)) {

    ## get input loss
    in_objective <- objective_function(y = Y,
                                       y_hat = NN_output(X = X,
                                                         NN_obj = iteration_input))

    ## iterate
    iteration_output <- GD_iter(NN_obj = iteration_input,
                                X = X,
```

```
                                Y = Y,
                                rho = rho,
                                verbose = FALSE,
                                very_verbose = FALSE)

    ## outputs
    out_objective <- objective_function(y = Y,
                                        y_hat = NN_output(X = X,
                                                          NN_obj = iteration_output))

    iteration_input <- iteration_output
    iteration_outputs[[iter]] <- iteration_output
    output_objectives[[iter]] <- out_objective

    if (print_descent == TRUE) {
      print(paste0("iter: ", iter, "; obj: ", round(out_objective, 1)))
    }

    iter <- iter + 1

    ## evaluate
    if (abs(in_objective - out_objective) < threshold) {
      done_decreasing <- TRUE
    }

  }

  return(list(final_NN = iteration_output,
              intermediate_NN = iteration_outputs,
              output_objectives = output_objectives,
              initial_objective = initial_objective,
              params = list(rho = rho,
                            loss_function = loss_function,
                            initial_NN = init_NN_obj)))
}
```

Summary Functions

```
GD_plot <- function(GD_obj) {

    data.frame(x = 1:length(GD_obj$output_objectives),
               y = GD_obj$output_objectives) %>%
    ggplot(aes(x = x,
               y = y)) +
    geom_point() +
    theme_bw() +
    labs(x = "Iteration",
         y = "Loss")

}

GD_summary <- function(GD_obj,
```

```
                     print_summary = TRUE) {

  ## num iter
  num_iter <- length(GD_obj$output_objectives)

  ## loss improvement
  initial_objective <- GD_obj$initial_objective %>% round(1)
  final_objective <- last(GD_obj$output_objectives) %>% round(1)
  loss_improvement_ratio <- (final_objective / initial_objective)  %>% round(4)

  if (print_summary == TRUE) {

    ## prints
    cat(paste0("Gradient Descent Summary:", "\n",
               "  |", "\n",
               "  |  Number of Iterations: ", num_iter, "\n",
               "  |", "\n",
               "  |  Initial Objective: ", initial_objective, "\n",
               "  |  Final Objective: ", final_objective, "\n",
               "  |  Ratio: ", loss_improvement_ratio, "\n", "\n"))

    cat(paste0("----------------------------------------", "\n",
               "Initial W:", "\n", "\n"))
    print(GD_obj$params$initial_NN$W[-1])
    cat(paste0("----------------------------------------", "\n",
               "Final W:", "\n", "\n"))
    print(GD_obj$final_NN$W[-1])

    cat(paste0("----------------------------------------", "\n",
               "Initial b:", "\n", "\n"))
    print(GD_obj$params$initial_NN$b[-1])
    cat(paste0("----------------------------------------", "\n",
               "Final b:", "\n", "\n"))
    print(GD_obj$final_NN$b[-1])

  }

  return(list(num_iter = num_iter,
              initial_objective = initial_objective,
              final_objective = final_objective,
              loss_improvement_ratio = loss_improvement_ratio))
}
```

Test

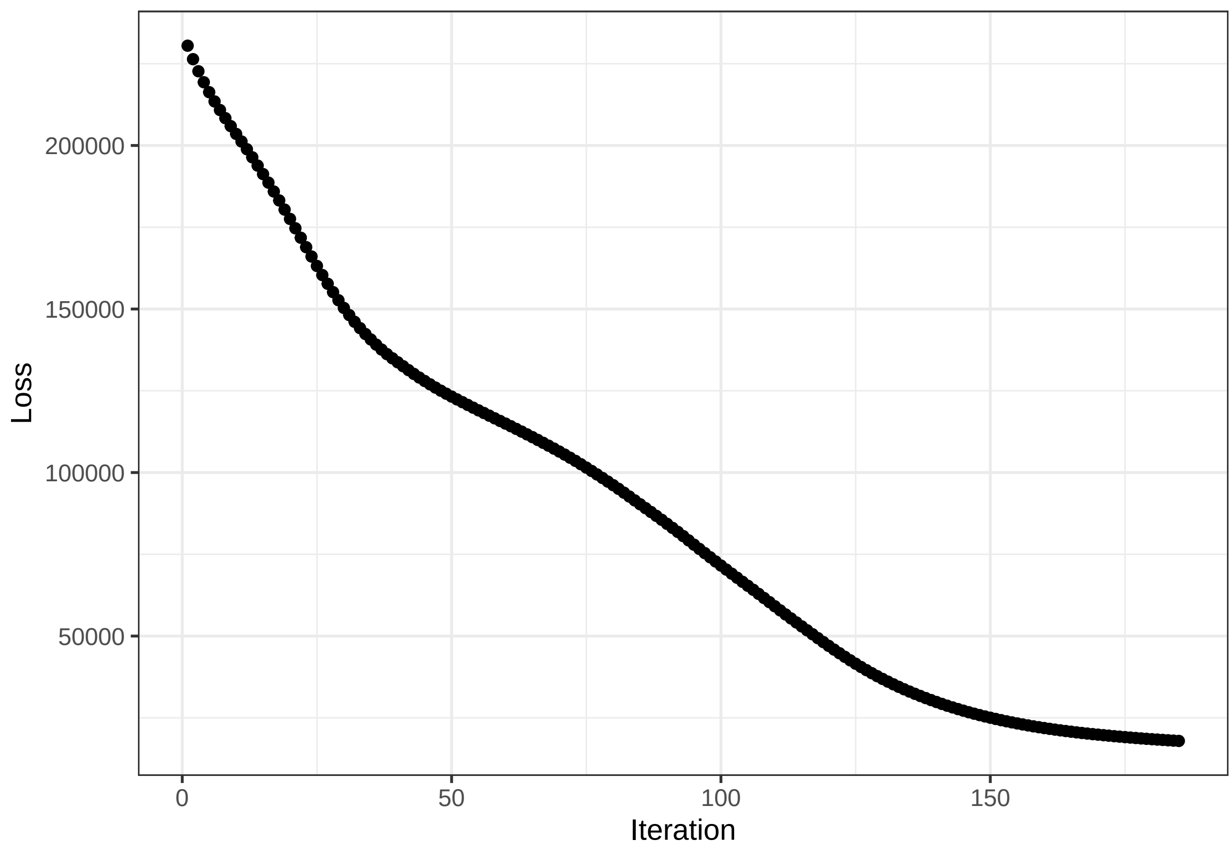
```
## initialize NN
init_NN <- initialize_NN(layer_sizes = c(3, 3, 1),
                         activation_function = "relu",
                         last_activation_function = "identity",
                         lower_bound = 0,
                         upper_bound = 1)
```

```r
## train NN
GD_NN <- GD_perform(X = X,
                    Y = Y,
                    init_NN_obj = init_NN,
                    rho = 0.001,
                    loss_function = "squared_error",
                    threshold = 100,
                    max_iter = 1000,
                    print_descent = FALSE)

final_NN <- GD_NN$final_NN

## Summaries
NN_sum <- GD_summary(GD_obj = GD_NN)
```

```
## Gradient Descent Summary:
##   |
##   |  Number of Iterations: 185
##   |
##   |  Initial Objective: 235117.1
##   |  Final Objective: 17941.5
##   |  Ratio: 0.0763
##
## ----------------------------------------
## Initial W:
##
## [[1]]
##           [,1]      [,2]      [,3]
## [1,] 0.7018891 0.6591868 0.8192264
## [2,] 0.2791028 0.2493214 0.4875481
## [3,] 0.9007776 0.3005512 0.3869135
##
## [[2]]
##           [,1]       [,2]     [,3]
## [1,] 0.7098611 0.06823424 0.474624
##
## ----------------------------------------
## Final W:
##
## [[1]]
##               X1          X2       X3
## [1,]  0.17036987  0.02720998 2.478817
## [2,] -0.03494768  0.04027869 1.261541
## [3,]  0.67616254 -0.14454166 1.415086
##
## [[2]]
##          [,1]     [,2]     [,3]
## [1,] 2.390102 1.217769 1.314926
##
## ----------------------------------------
## Initial b:
##
## [[1]]
```

```
##             [,1]
## [1,] 0.49964774
## [2,] 0.56574421
## [3,] 0.01850559
##
## [[2]]
##           [,1]
## [1,] 0.3447208
##
## ----------------------------------------
## Final b:
##
## [[1]]
##           [,1]
## [1,] 0.9432974
## [2,] 0.7618366
## [3,] 0.3126433
##
## [[2]]
##           [,1]
## [1,] 0.8748807
```

```
GD_plot(GD_NN)
```



Next Steps

In the future:

- need some sort of divergence check / pick 'best so far' output
- vis for gradient descent — pick 2 vars and for every combo of those 2, plot the objective function
- vis for gradient descent — show the evolution of the var through gradient descent over iterations
- NN overall vis & perhaps animation
- multi-dimensional output (cat / 1-hot)
- different cost functions (softmax squared-error & cross-entropy)
- 'from scratch' from scratch — mmult and maybe further lol
- get 'best-case' / perfect objective function (if data creation process known)
- stochastic gradient descent, minibatches (what gets passed down to GD_iter from GD_perform)
- regularization methods & CV-validation

```r
## get_layer_size function
get_layer_sizes <- function(NN_obj) {
  n_1 <- ncol(NN_obj$W[[2]])

  n_H <- sapply(NN_obj$W[-1],
                nrow)

  return(c(n_1, n_H))
}
```

```r
layer_sizes_test <- get_layer_sizes(final_NN)
```