model

In [1]:
```
class NeuralNetMLP(object):
    def __init__(self, is_sigmoid=True, initializer=None, dropout_rate=1., n_laye
                 n_hidden=5, l2=0., epochs=100, eta=0.0005, shuffle=True,\
                 minibatch_size=64, seed=666):
        self.random = np.random.RandomState(seed)
        self.is_sigmoid = is_sigmoid
        self.initializer = initializer
        self.dropout_rate = dropout_rate
        self.n_layers = n_layers
        self.n_hidden = n_hidden
        self.l2 = l2
        self.epochs = epochs
        self.eta = eta
        self.shuffle = shuffle
        self.minibatch_size = minibatch_size
        self.k = locals()
        if n_layers < 3:
            raise Exception("n_layers must be >= 3 !!!")
    def _onehot(self, y, n_classes):
        """Encode labels into one-hot representation
        Parameters
        ------------
        y : array, shape = [n_samples]
        Target values.
        Returns
        -----------
        onehot : array, shape = (n_samples, n_labels)
        """
        onehot = np.zeros((n_classes, y.shape[0]))
        for idx, val in enumerate(y.astype(int)):
            onehot[val, idx] = 1.
        return onehot.T
    def _sigmoid(self, z):
        """Compute logistic function (sigmoid)"""
        return 1. / (1. + np.exp(-np.clip(z, -250, 250)))
    def _forward(self, X, is_training=True):
        """Compute forward propagation step"""
            # step 1: net input of hidden layer
        if is_training:
            dropout_rate = self.dropout_rate
        else:
            dropout_rate = 1.
        for i in range(self.n_layers - 2):
            if i == 0:
                # [n_samples, n_features] dot [n_features, n_hidden]
                # -> [n_samples, n_hidden]
                r = self.random.binomial(1, dropout_rate, size=X.shape)
                X = r * X
                self.k['z_h_{}'.format(i+1)] = \
                np.dot(X, self.k['w_h_{}'.format(i+1)]) + self.k['b_h_{}'.format(
                # step 2: activation of hidden layer
                if self.is_sigmoid:
                    self.k['a_h_{}'.format(i+1)] = self._sigmoid(self.k['z_h_{}'.
                else:
                    self.k['a_h_{}'.format(i+1)] = self.k['z_h_{}'.format(i+1)]
            else:
```

```
            # [n_samples, n_hidden] dot [n_hidden, n_hidden]
            # -> [n_samples, n_hidden]
            r = self.random.binomial(1, dropout_rate, size=self.k['a_h_{}'.fo
            self.k['a_h_{}'.format(i)] = r * self.k['a_h_{}'.format(i)]
            self.k['z_h_{}'.format(i+1)] = \
            np.dot(self.k['a_h_{}'.format(i)] , self.k['w_h_{}'.format(i+1)])
            + self.k['b_h_{}'.format(i+1)]
            # step 2: activation of hidden layer
            if self.is_sigmoid:
                self.k['a_h_{}'.format(i+1)] = self._sigmoid(self.k['z_h_{}'.
            else:
                self.k['a_h_{}'.format(i+1)] = self.k['z_h_{}'.format(i+1)]
        # step 3: net input of output layer
        # [n_samples, n_hidden] dot [n_hidden, n_classlabels]
        # -> [n_samples, n_classlabels]
        z_out = np.dot(self.k['a_h_{}'.format(self.n_layers - 2)], self.w_out) +
        # step 4: activation output layer
        if self.regression_problem:
            a_out = z_out
        else:
            a_out = self._sigmoid(z_out)
        return [self.k['z_h_{}'.format(i+1)] for i in range(self.n_layers - 2)],
    [self.k['a_h_{}'.format(i+1)] for i in range(self.n_layers - 2)], z_out, a_ou
    def _compute_cost(self, y_enc, output):
        """Compute cost function.
        Parameters
        ----------
        y_enc : array, shape = (n_samples, n_labels)
        one-hot encoded class labels.
        output : array, shape = [n_samples, n_output_units]
        Activation of the output layer (forward propagation)
        Returns
        ---------
        cost : float
        Regularized cost
        """
        L2_term = (self.l2 *
        (np.sum([np.sum(self.k['w_h_{}'.format(i+1)] ** 2.) for i in range(self.r
        np.sum(self.w_out ** 2.)))
        term1 = -y_enc * (np.log(output))
        term2 = (1. - y_enc) * np.log(1. - output)
        if not self.regression_problem:
            cost = np.sum(term1 - term2) + L2_term
        else:
            cost = np.sum((output - y_enc) ** 2. )
        return cost
    def predict(self, X):
        """Predict class labels
        Parameters
        -----------
        X : array, shape = [n_samples, n_features]
        Input layer with original features.
        Returns:
        ----------
        y_pred : array, shape = [n_samples]
        Predicted class labels.
        """
```

```
        z_h, a_h, z_out, a_out = self._forward(X, is_training=False)
        if self.regression_problem:
            y_pred = a_out
        else:
            y_pred = np.argmax(z_out, axis=1)
        return y_pred
    def R_square(self, output, targets):
#         n = len(targets)
#         MSE = (1 / n) * (np.sum((output - targets) ** 2))
#         rMSE = MSE / np.var(targets)
#         r_2 = 1 - rMSE
        return r2_score(targets, output)

    def fit(self, X_train, y_train, X_valid, y_valid):
        """ Learn weights from training data.
        Parameters
        -----------
        X_train : array, shape = [n_samples, n_features]
        Input layer with original features.
        y_train : array, shape = [n_samples]
        Target class labels.
        X_valid : array, shape = [n_samples, n_features]
        Sample features for validation during training
        y_valid : array, shape = [n_samples]
        Sample labels for validation during training
        Returns:
        ----------
        self
        """
        if np.sum(y_train % 1) == 0:
            n_output = np.unique(y_train).shape[0] # no. of class labels
            self.regression_problem = False
        else:
            n_output = 1
            self.regression_problem = True
        n_features = X_train.shape[1]
        ########################
        # Weight initialization
        ########################


        for i in range(self.n_layers - 2):
            # weights for input -> hidden
            self.k['b_h_{}'.format(i+1)] = np.zeros(self.n_hidden)
            if i == 0:
                if self.initializer == 'Xavier':
                    self.k['w_h_{}'.format(i+1)] = \
                    self.random.normal(loc=0.0, \
                                       scale=(2 / (n_features + self.n_hidden)) *
                                       , size=(n_features, self.n_hidden))
                else:
                    self.k['w_h_{}'.format(i+1)] = \
                    self.random.normal(loc=0.0, scale=0.1\
                                       , size=(n_features, self.n_hidden))

            else:
                if self.initializer == 'Xavier':
```

```
                    self.k['w_h_{}'.format(i+1)] = \
                    self.random.normal(loc=0.0, \
                                       scale=(2 / (self.n_hidden + self.n_hidden)
                                       , size=(self.n_hidden, self.n_hidden))
                else:
                    self.k['w_h_{}'.format(i+1)] = \
                    self.random.normal(loc=0.0, scale=0.1\
                                       , size=(self.n_hidden, self.n_hidden))
        # weights for hidden -> output
        if self.regression_problem:
            self.b_out = np.ones(n_output) * np.mean(y_train)
        else:
            self.b_out = np.zeros(n_output)
        if self.initializer == 'Xavier':
            self.w_out = self.random.normal(loc=0.0, \
                                            scale=(2 / (self.n_hidden + n_output)
                                            size=(self.n_hidden, n_output))
        else:
            self.w_out = self.random.normal(loc=0.0, scale=0.1, \
                                            size=(self.n_hidden, n_output))

        epoch_strlen = len(str(self.epochs)) # for progr. format.
        self.eval_ = {'cost': [], 'train_acc': [], 'valid_acc': []}
        if not self.regression_problem:
            y_train_enc = self._onehot(y_train, n_output)
        else:
            y_train_enc = y_train
        # iterate over training epochs
        for i in range(self.epochs):
            # iterate over minibatches
            indices = np.arange(X_train.shape[0])
            if self.shuffle:
                self.random.shuffle(indices)
            for start_idx in range(0, \
                indices.shape[0] -self.minibatch_size +1, \
                self.minibatch_size):
                batch_idx = indices\
                [start_idx:start_idx+self.minibatch_size]
                # forward propagation
                # z_h: list(z_h_1, z_h_2, ......)
                z_h, a_h, z_out, a_out = \
                self._forward(X_train[batch_idx])
                ##################
                # Backpropagation
                ##################
                # [n_samples, n_classlabels]
                sigma_out = a_out - y_train_enc[batch_idx]

                for l in range(self.n_layers - 2):
                    # [n_samples, n_hidden]
                    # a_h: list(a_h_1, a_h_2, ......)
                    sigmoid_derivative_h = a_h[-1-l] * (1. - a_h[-1-l])
                    # [n_samples, n_classlabels] dot
                    # [n_classlabels, # n_hidden]
                    # -> [n_samples, n_hidden]
                    if l == 0:
#                         if self.regression_problem:
```

```
#                               self.k['sigma_h_{}'.format(self.n_layers-2-l)] = \
#                               (np.dot(sigma_out, self.w_out.T))
#                           else:
#                               self.k['sigma_h_{}'.format(self.n_layers-2-l)] = \
#                               (np.dot(sigma_out, self.w_out.T) * sigmoid_derivati
                        if self.is_sigmoid:
                            self.k['sigma_h_{}'.format(self.n_layers-2-l)] = \
                            (np.dot(sigma_out, self.w_out.T) * sigmoid_derivative
                        else:
                            self.k['sigma_h_{}'.format(self.n_layers-2-l)] = \
                            (np.dot(sigma_out, self.w_out.T))
                    else:
                        if self.is_sigmoid:
                            self.k['sigma_h_{}'.format(self.n_layers-2-l)] = \
                            (np.dot(self.k['sigma_h_{}'.format(self.n_layers-1-l)
                                    self.k['w_h_{}'.format(self.n_layers-1-l)].T)
                             sigmoid_derivative_h)
                        else:
                            self.k['sigma_h_{}'.format(self.n_layers-2-l)] = \
                            (np.dot(self.k['sigma_h_{}'.format(self.n_layers-1-l)
                                    self.k['w_h_{}'.format(self.n_layers-1-l)].T)

                for l in range(2, self.n_layers - 1):
                        # [n_features, n_samples] dot [n_samples, n_hidden]
                        # -> [n_features, n_hidden]
                        self.k['grad_w_h_{}'.format(l)] = np.dot(a_h[l-2].T, self
                        self.k['grad_b_h_{}'.format(l)] = np.sum(self.k['sigma_h_
                # [n_features, n_samples] dot [n_samples, n_hidden]
                # -> [n_features, n_hidden]
                self.k['grad_w_h_1'] = np.dot(X_train[batch_idx].T, self.k['sigma
                self.k['grad_b_h_1'] = np.sum(self.k['sigma_h_1'], axis=0)
                # [n_hidden, n_samples] dot [n_samples, n_classlabels]
                # -> [n_hidden, n_classlabels]
                grad_w_out = np.dot(a_h[-1].T, sigma_out)
                grad_b_out = np.sum(sigma_out, axis=0)



                # Regularization and weight updates
                for l in range(self.n_layers - 2):
                    self.k['delta_w_h_{}'.format(l+1)] = (self.k['grad_w_h_{}'.fo
                                                          self.l2*self.k['w_h_{}'.format
                    self.k['delta_b_h_{}'.format(l+1)] = self.k['grad_b_h_{}'.for
                    self.k['w_h_{}'.format(l+1)] -= self.eta * self.k['delta_w_h_
                    self.k['b_h_{}'.format(l+1)] -= self.eta * self.k['delta_b_h_
                delta_w_out = (grad_w_out + self.l2*self.w_out)
                delta_b_out = grad_b_out # bias is not regularized
                self.w_out -= self.eta * delta_w_out
                self.b_out -= self.eta * delta_b_out
            #############
            # Evaluation
            #############
            # Evaluation after each epoch during training
            z_h, a_h, z_out, a_out = self._forward(X_train)
            cost = self._compute_cost(y_train_enc,a_out)
            y_train_pred = self.predict(X_train)
            y_valid_pred = self.predict(X_valid)
```

```
                if not self.regression_problem:
                    train_acc = ((np.sum(y_train == \
                    y_train_pred)).astype(np.float) /
                    X_train.shape[0])
                    valid_acc = ((np.sum(y_valid ==\
                    y_valid_pred)).astype(np.float) /
                    X_valid.shape[0])
                else:
                    train_acc = self.R_square(output=y_train_pred, targets=y_train)
                    valid_acc = self.R_square(output=y_valid_pred, targets=y_valid)
                self.eval_['cost'].append(cost)
                self.eval_['train_acc'].append(train_acc)
                self.eval_['valid_acc'].append(valid_acc)
#          return self
    def get_weights(self):
        for i in range(self.n_layers - 2):
            print('w_h_{}: {}'.format(i + 1, self.k['w_h_{}'.format(i + 1)].shape
                   self.k['w_h_{}'.format(i + 1)])
        print('w_out: {}'.format(self.w_out.shape), self.w_out)
    def get_loss_plot(self):
        plt.plot(range(self.epochs), self.eval_['cost'])
        plt.ylabel('Cost')
        plt.xlabel('Epochs')
        plt.show()
```

In [2]:

```
import warnings
warnings.filterwarnings('ignore')
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from sklearn.metrics import r2_score
```

data

In [3]:
```python
from sklearn.datasets import load_boston
X, y = load_boston(return_X_y=True)
boston = load_boston()
print(boston.DESCR)
```

```
.. _boston_dataset:

Boston house prices dataset
---------------------------

**Data Set Characteristics:**

    :Number of Instances: 506

    :Number of Attributes: 13 numeric/categorical predictive. Median Value (att
ribute 14) is usually the target.

    :Attribute Information (in order):
        - CRIM     per capita crime rate by town
        - ZN       proportion of residential land zoned for lots over 25,000 s
q.ft.
        - INDUS    proportion of non-retail business acres per town
        - CHAS     Charles River dummy variable (= 1 if tract bounds river; 0 o
therwise)
        - NOX      nitric oxides concentration (parts per 10 million)
        - RM       average number of rooms per dwelling
        - AGE      proportion of owner-occupied units built prior to 1940
        - DIS      weighted distances to five Boston employment centres
        - RAD      index of accessibility to radial highways
        - TAX      full-value property-tax rate per $10,000
        - PTRATIO  pupil-teacher ratio by town
        - B        1000(Bk - 0.63)^2 where Bk is the proportion of blacks by to
wn
        - LSTAT    % lower status of the population
        - MEDV     Median value of owner-occupied homes in $1000's

    :Missing Attribute Values: None

    :Creator: Harrison, D. and Rubinfeld, D.L.

This is a copy of UCI ML housing dataset.
https://archive.ics.uci.edu/ml/machine-learning-databases/housing/ (https://arc
hive.ics.uci.edu/ml/machine-learning-databases/housing/)


This dataset was taken from the StatLib library which is maintained at Carnegie
Mellon University.

The Boston house-price data of Harrison, D. and Rubinfeld, D.L. 'Hedonic
prices and the demand for clean air', J. Environ. Economics & Management,
vol.5, 81-102, 1978.   Used in Belsley, Kuh & Welsch, 'Regression diagnostics
...', Wiley, 1980.   N.B. Various transformations are used in the table on
pages 244-261 of the latter.

The Boston house-price data has been used in many machine learning papers that
 address regression
```

```
problems.

.. topic:: References

   - Belsley, Kuh & Welsch, 'Regression diagnostics: Identifying Influential Da
ta and Sources of Collinearity', Wiley, 1980. 244-261.
   - Quinlan,R. (1993). Combining Instance-Based and Model-Based Learning. In P
roceedings on the Tenth International Conference of Machine Learning, 236-243,
 University of Massachusetts, Amherst. Morgan Kaufmann.
```

In [4]:

```
df = pd.DataFrame(X, columns=boston.feature_names)
df.head(2)
```

Out[4]:

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	B	LSTAT
0	0.00632	18.0	2.31	0.0	0.538	6.575	65.2	4.0900	1.0	296.0	15.3	396.9	4.98
1	0.02731	0.0	7.07	0.0	0.469	6.421	78.9	4.9671	2.0	242.0	17.8	396.9	9.14

In [5]:

```
df.describe()
```

Out[5]:

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	
count	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.00
mean	3.613524	11.363636	11.136779	0.069170	0.554695	6.284634	68.574901	3.79
std	8.601545	23.322453	6.860353	0.253994	0.115878	0.702617	28.148861	2.10
min	0.006320	0.000000	0.460000	0.000000	0.385000	3.561000	2.900000	1.12
25%	0.082045	0.000000	5.190000	0.000000	0.449000	5.885500	45.025000	2.10
50%	0.256510	0.000000	9.690000	0.000000	0.538000	6.208500	77.500000	3.20
75%	3.677083	12.500000	18.100000	0.000000	0.624000	6.623500	94.075000	5.18
max	88.976200	100.000000	27.740000	1.000000	0.871000	8.780000	100.000000	12.12

In [6]:

```
f_dummy = np.array(df['CHAS'])[:, np.newaxis]
del df['CHAS']
f = np.array(df)
```

In [7]:

```
from sklearn.preprocessing import StandardScaler
scalar = StandardScaler()
f = scalar.fit_transform(f)

X = np.concatenate((f, f_dummy), axis=1)
X.shape
```

Out[7]: (506, 13)

In [8]:
```
split_idx = int(len(X) * 0.9)
y = y[:, np.newaxis]
X_train, X_test = X[:split_idx], X[split_idx:]
y_train, y_test = y[:split_idx], y[split_idx:]
```

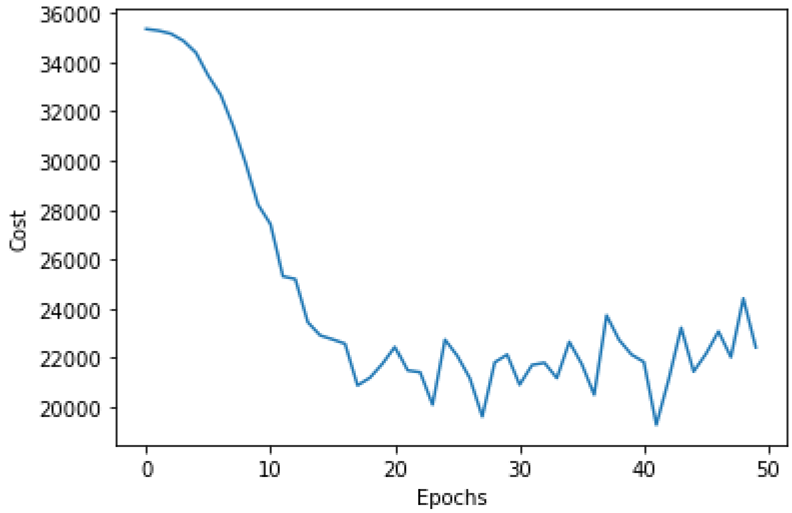
train

In [9]:
```
idx = int(len(X_train) * 0.9)
nn = NeuralNetMLP(epochs=50,dropout_rate=0.5, n_hidden=5, n_layers=3,minibatch_si
nn.fit(X_train=X_train[:idx],\
y_train=y_train[:idx],\
X_valid=X_train[idx:],\
y_valid=y_train[idx:])
```

In [10]:
```
nn.get_weights()
```

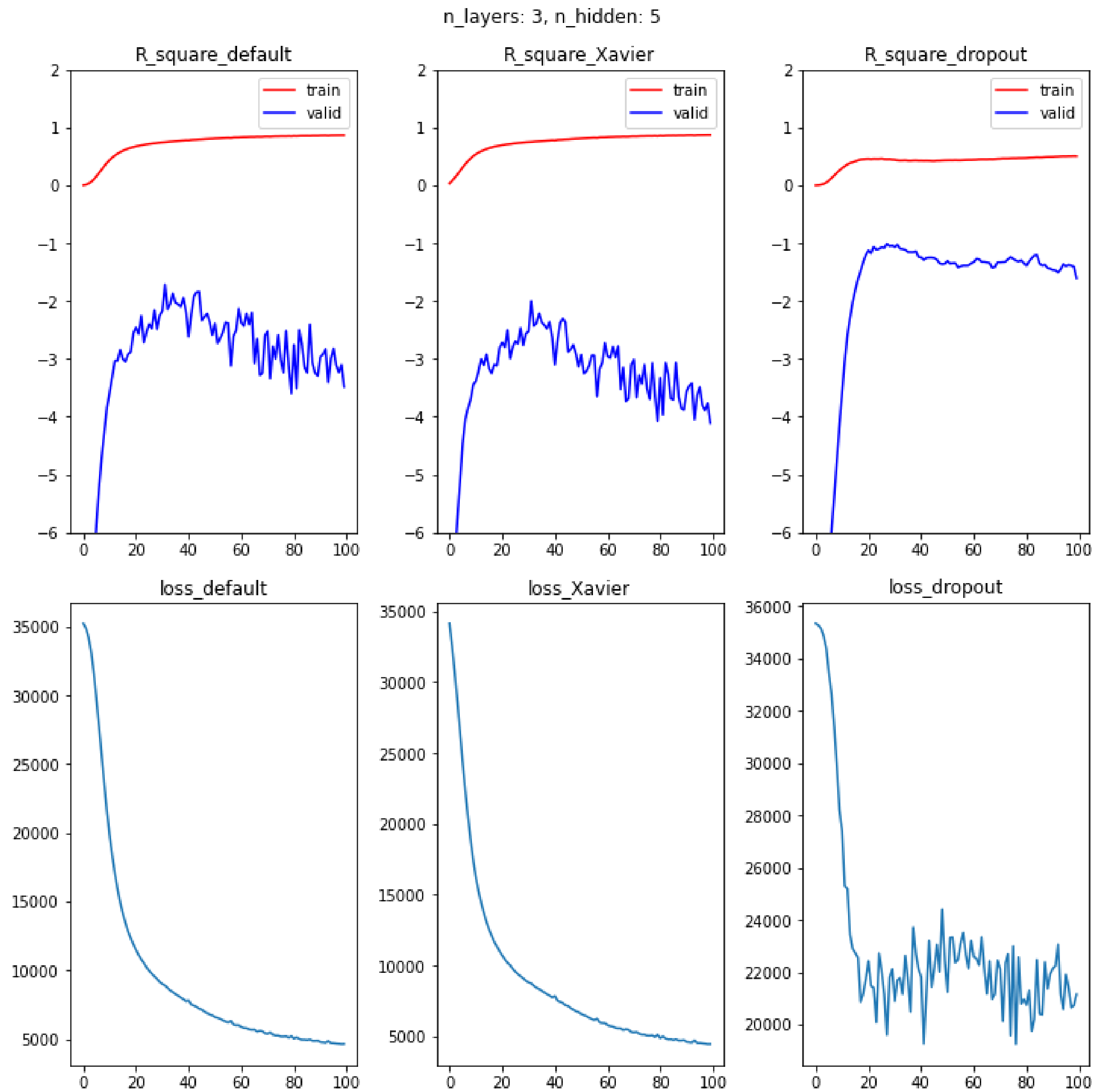
```
w_h_1: (13, 5) [[ 0.91465083  1.02677732 -0.9625498  -0.86549987 -1.06891682]
 [-1.21793391 -1.08328517  0.95387523  1.35420732  0.98387599]
 [ 1.17331028  1.08411514 -1.17962309 -1.29020613 -1.33110834]
 [ 0.497263    0.74107993 -1.10802003 -0.90549064 -1.04737985]
 [-8.7014977  -6.9412538   6.40470926  7.88121075  6.3499206 ]
 [ 0.17936506  0.64279604 -0.81606997 -0.37955351 -0.79747339]
 [ 2.27258802  1.59794487 -1.09993141 -1.95366368 -1.00514567]
 [-1.12869033 -0.57984266  0.24115697  0.87340431  0.36835915]
 [ 0.25562907  0.72781903 -0.74809453 -0.46790867 -0.79915811]
 [ 2.40805552  2.42575578 -2.17382311 -2.6261473  -1.94778534]
 [-0.16453019 -0.13731082  0.39379391  0.17459239  0.49863058]
 [ 5.78599162  4.96261853 -4.93909243 -5.50816472 -4.71470803]
 [-0.89176109 -0.1819256   0.49315658  0.43121306  0.5519309 ]]
w_out: (5, 1) [[-3.31570253]
 [-2.58439414]
 [ 2.41904997]
 [ 2.94974384]
 [ 2.42346269]]
```

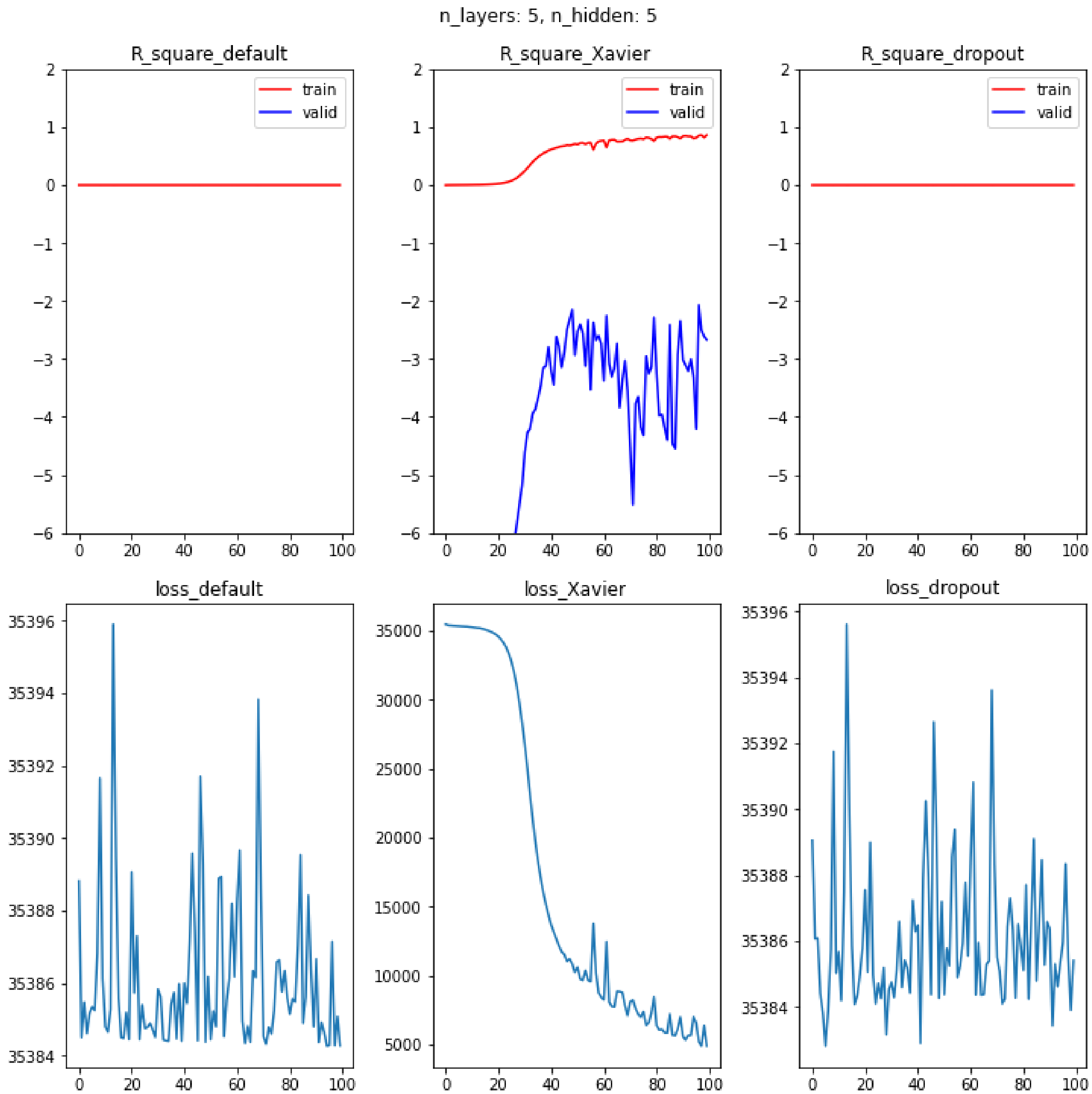
In [11]:
```
nn.get_loss_plot()
```

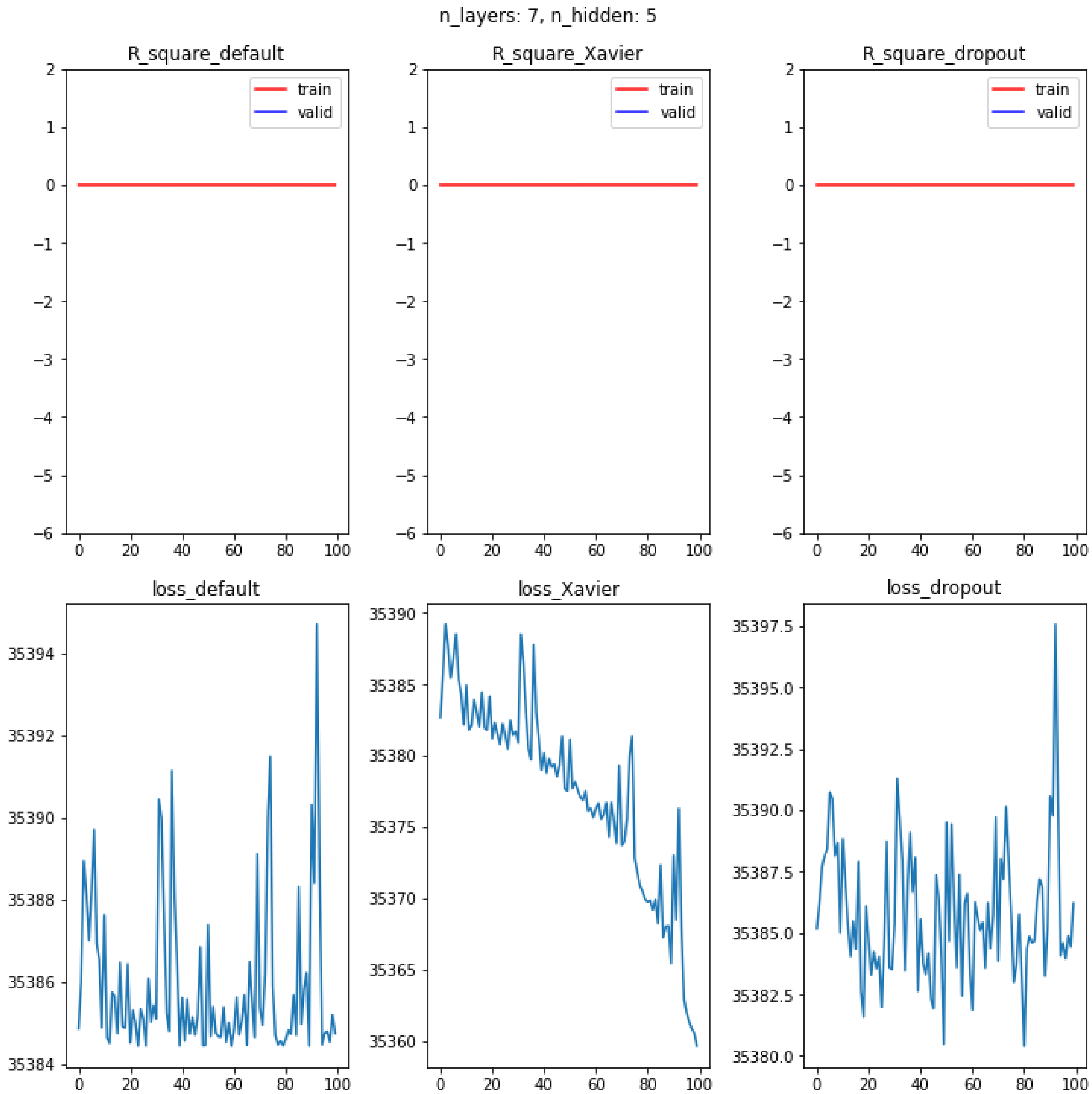


In [12]:
```
kk = locals()
n_models = 3
def nns(X_train, y_train, fig, axs, is_sigmoid=True, dropout_rate=0.8, n_layers=3
    if is_sigmoid:
        kk['nn_0'] = NeuralNetMLP(n_layers=n_layers)
        kk['nn_1'] = NeuralNetMLP(initializer='Xavier', n_layers=n_layers)
        kk['nn_2'] = NeuralNetMLP(dropout_rate=dropout_rate, n_layers=n_layers)
    else:
        kk['nn_0'] = NeuralNetMLP(is_sigmoid=False, n_layers=n_layers)
        kk['nn_1'] = NeuralNetMLP(is_sigmoid=False, initializer='Xavier', n_layer
        kk['nn_2'] = NeuralNetMLP(is_sigmoid=False, dropout_rate=dropout_rate, n_
    for i in range(n_models):
        kk['nn_{}'.format(i)].fit(X_train=X_train[:idx],\
        y_train=y_train[:idx],\
        X_valid=X_train[idx:],\
        y_valid=y_train[idx:])

    title = ['default', 'Xavier', 'dropout']

    col = ['red', 'blue']
    label = ['train', 'valid']


    for i in range(n_models):
        acc = [kk['nn_{}'.format(i)].eval_['train_acc'], \
              kk['nn_{}'.format(i)].eval_['valid_acc']]
        axs[0, i].set_title('R_square_' + title[i])
        axs[0, i].set_ylim([-6, 2])
        for l in range(len(col)):
            axs[0, i].plot(acc[l], color=col[l], label=label[l])
            axs[0, i].legend(frameon=True)
        axs[1, i].set_title('loss_' + title[i])
        axs[1, i].plot(range(kk['nn_{}'.format(i)].epochs), \
                    kk['nn_{}'.format(i)].eval_['cost'])
    fig.suptitle('n_layers: {}, n_hidden: {}'.format(n_layers, nn_0.n_hidden))
    return fig
```

In [13]:
```
n_n_layers = 3
for i in range(n_n_layers):
    n_layers = 3 + i*2
    kk['fig_{}'.format(i)], kk['axs_{}'.format(i)] = \
    plt.subplots(2, n_models, constrained_layout=True, figsize = (10, 10))
    kk['fig_{}'.format(i)] = nns(X_train, y_train, kk['fig_{}'.format(i)], kk['ax
                                  , is_sigmoid=True, dropout_rate=0.5, n_layers=n_
```




n_layers: 5, n_hidden: 5
R_square_default
R_square_Xavier
R_square_dropout
train
valid
loss_default
loss_Xavier
loss_dropout



In [14]:
```
y_fake = nn_0.predict(X_train) + np.random.normal(0, 1, y_train.shape)
```

In [15]:
```
nn_0.predict(X_train)
```

```
       [24.02514305],
       [24.02514302],
       [24.02514303],
       [24.02514304],
       [24.02514305],
       [24.02514305],
       [24.02514305],
       [24.02514305],
       [24.02514309],
       [24.0251431 ],
       [24.02514308],
       [24.02514307],
       [24.02514307],
       [24.02514306],
       [24.02514306],
       [24.02514305],
       [24.02514305],
       [24.02514301],
       [24.02514305],
       [24.02514306],
```

In [16]:
```
y_fake
```

```
       [23.61092158],
       [23.92484121],
       [24.04835094],
       [24.43245537],
       [24.74404654],
       [22.28661864],
       [23.30150156],
       [23.90328032],
       [23.64474879],
       [22.88075889],
       [24.48316083],
       [25.86448235],
       [23.48361724],
       [23.90861607],

       [25.91920143],
       [24.75466232],
       [24.30764747],
       [24.05531628],
       [25.84156892],
```

In [17]:
```
n_n_layers = 3
for i in range(n_n_layers):
    n_layers = 3 + i*2
    kk['fig_{}'.format(i)], kk['axs_{}'.format(i)] = \
    plt.subplots(2, n_models, constrained_layout=True, figsize = (10, 10))
    kk['fig_{}'.format(i)] = nns(X_train, y_fake, kk['fig_{}'.format(i)], kk['axs
                                 , is_sigmoid=False, dropout_rate=0.5, n_layers=n
```