CS5489 - Machine Learning

Lecture 8b - Neural Networks

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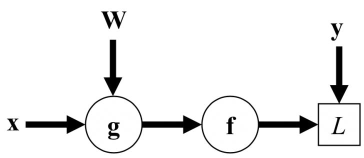
Outline

- History
- Perceptron
- Multi-class logistic regression
- **Multi-layer perceptron (MLP)**

Extracting features

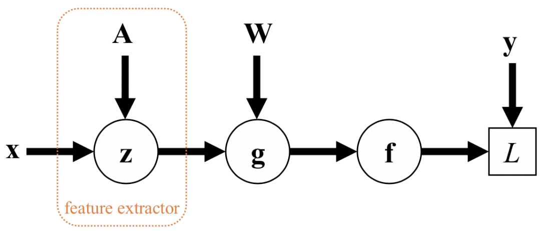
- The multi-class logistic regression model assumes the inputs are feature vectors.
  - $\mathbf{g} = \mathbf{W}^T\mathbf{x}$
  - $\mathbf{f} = \mathbf{s}(\mathbf{g})$



- What if we also want to learn the feature vectors?
  - Replace $\mathbf{x}$ with a feature extractor.
  - For simplicity, we can reuse the same "unit" as the classifier to compute the "features".

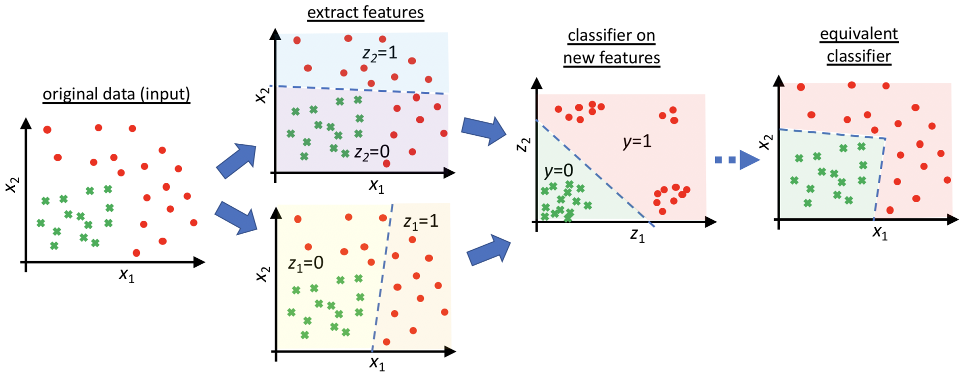
- Replace $\mathbf{x}$ with feature extractor $\mathbf{z} = \sigma(\mathbf{A}^T\mathbf{x})$
  - $\mathbf{z}$ is the extracted feature vector (also called *hidden* nodes)
    - $z_i = \sigma(\mathbf{a}_i^T\mathbf{x})$ is a hidden node.
  - $\sigma()$ is the sigmoid function (also called *activation* function.)
  - $\mathbf{A}$ are the parameters of the feature extractor.

- New model
  - $\mathbf{z} = \sigma(\mathbf{A}^T\mathbf{x})$
  - $\mathbf{g} = \mathbf{W}^T\mathbf{z}$
  - $\mathbf{f} = \mathbf{s}(\mathbf{g})$



- **Interpretation**
  - Each hidden node z_i is a "classifier" looking for pattern based on $\mathbf{a}_i$.

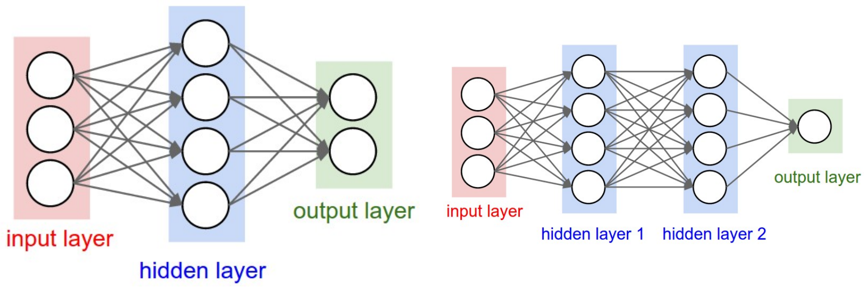
- The output is looking for patterns in the vector $\mathbf{x}$
- the effect is a non-linear classifier in the input space of $\mathbf{x}$.



- we can apply this recursively to create features of features

Multi-layer Perceptron

- Add hidden layers between the inputs and outputs
  - each hidden node is a Perceptron (with its own set of weights)
    - its inputs are the outputs from previous layer
    - extracts a feature pattern from the previous layer
  - can model more complex functions



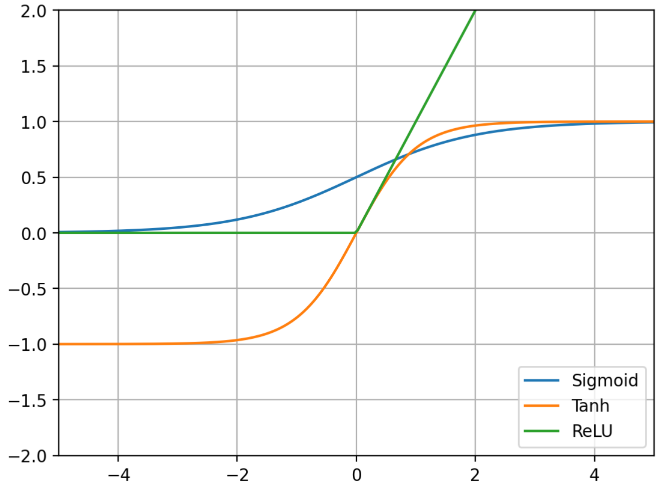
- Formally, for one layer:
  - $\mathbf{h} = f(\mathbf{W}^T\mathbf{x})$
    - Weight matrix $\mathbf{W}$ - one column for each node
    - Input $\mathbf{x}$ - from previous layer
    - Output $\mathbf{h}$ - to next layer
    - $f(a)$ is the activation function - applied to each dimension to get output
- Also called *fully-connected layers* or *dense layers*

Activation functions

- There are different types of activation functions:
  - *Sigmoid* - output [0,1]
  - *Tanh* - output [-1,1]
  - *Rectifier Linear Unit (ReLU)* - output [0,∞]

In [3]:
```
actfig
```

Out[3]:



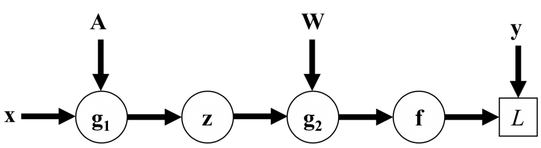
- Activation functions specifically for output nodes:
  - *Linear* - output for regression
  - *Softmax* - output for classification (same as multi-class logistic regression)
- Each layer can use a different activation function.

Which activation function is best?

- In the early days, only the Sigmoid and Tanh activation functions were used.
  - these were notoriously hard to train with.
    - gradient decays to zero on both ends
- Recently, ReLU has become very popular.
  - easier to train with - gradient is either 0 or 1.
  - faster - don't need to calculate exponential
  - sparse representation - most nodes will output zero.

Training an MLP

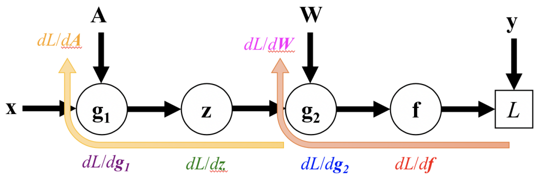
- Assume a general case:
  - linear transform: $\mathbf{g}_1 = \mathbf{A}^T\mathbf{x}$
  - activation: $\mathbf{z} = h_1(\mathbf{g}_1)$
  - linear transform: $\mathbf{g}_2 = \mathbf{W}^T\mathbf{z}$
  - activation: $\mathbf{f} = h_2(\mathbf{g}_2)$
  - loss function: $L(\mathbf{y}, \mathbf{f})$



- In our example, h_1 is a sigmoid, h_2 is a softmax.

- Similar to multi-class logistic regression
  - minimize the loss
    - $(\mathbf{A}^*, \mathbf{W}^*) = \text{argmin}_{\mathbf{A},\mathbf{W}} L(\mathbf{y}, \mathbf{f}(\mathbf{x}))$
  - use gradient descent as before
    - need to compute $\frac{dL}{d\mathbf{A}}$ and $\frac{dL}{d\mathbf{W}}$
    - we have done most of the work already...

- Computation graph

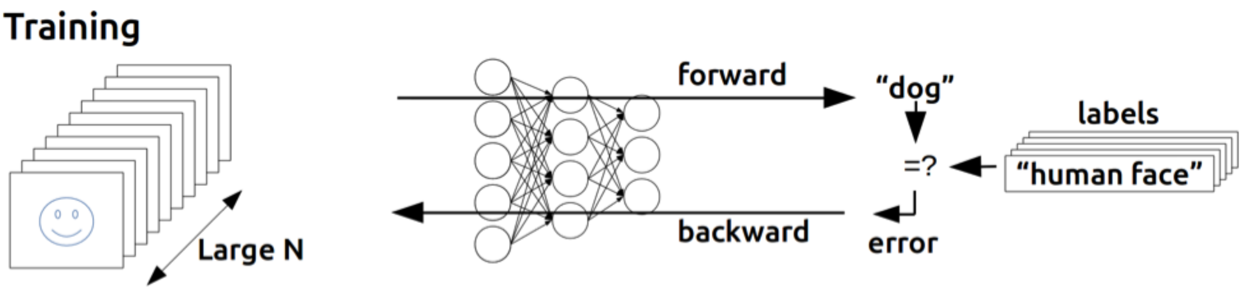


- Chain rule:
  - 1. $\frac{dL}{d\mathbf{f}}$
  - 2. $\frac{dL}{d\mathbf{g}_2} = \frac{d\mathbf{f}^T}{d\mathbf{g}_2}\frac{dL}{d\mathbf{f}} \Rightarrow$ 3) $\frac{dL}{d\mathbf{w}_j} = \frac{d\mathbf{g}_2^T}{d\mathbf{w}_j}\frac{dL}{d\mathbf{g}_2}$
  - 4. $\frac{dL}{d\mathbf{z}} = \frac{d\mathbf{g}_2^T}{d\mathbf{z}}\frac{dL}{d\mathbf{g}_2}$
  - 5. $\frac{dL}{d\mathbf{g}_1} = \frac{d\mathbf{z}^T}{d\mathbf{g}_1}\frac{dL}{d\mathbf{z}} \Rightarrow$ 6) $\frac{dL}{d\mathbf{a}_j} = \frac{d\mathbf{g}_1^T}{d\mathbf{a}_j}\frac{dL}{d\mathbf{g}_1}$

- Recursively use the gradient of descendant layers
  - propagate gradient backwards
  - backwards propagation
  - back propagation
  - backpropagation
  - backprop
  - BP

Backpropagation (backward propagation)

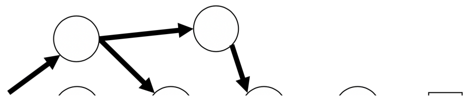
- Defines a set of recursive relationships
  1. calculate the output of each node from first to last layer
  2. calculate the gradient of each node from last to first layer



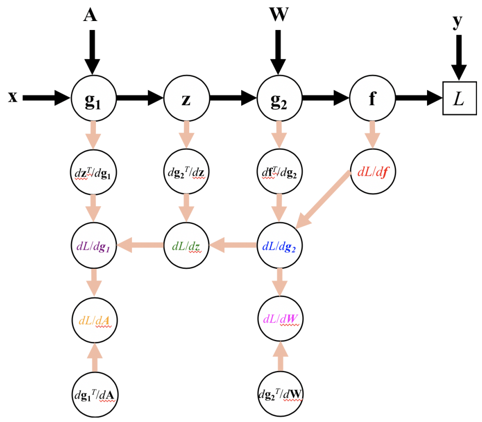
- **NOTE:** the gradients multiply in each layer!
  - if two gradients are small (<1), their product will be even smaller. This is the "vanishing gradient" problem.

Backpropagation (general form)

- Given a computation graph
  1. apply input $\mathbf{x}$ and forward propagate to compute all the nodes' values and the loss.
  2. Go backwards from end, at node $\mathbf{h}$:
  - compute gradients from child nodes: $\frac{dL}{d\mathbf{h}} = \sum_{g \in \text{child}(\mathbf{h})} \frac{d\mathbf{g}^T}{d\mathbf{h}}\frac{dL}{d\mathbf{g}}$
  - compute gradient of parameters $\mathbf{w}_h$ of h: $\frac{dL}{d\mathbf{w}_h} = \frac{d\mathbf{h}^T}{d\mathbf{w}_h}\frac{dL}{d\mathbf{h}}$
- This is the "symbol-to-number" differentiation (e.g., Caffe, Torch).



- We can also make the backprop operations as part of the computation graph.
  - called "symbol-to-symbol" differentiation (e.g., Tensorflow, Theano)



Stochastic Gradient Descent (SGD)

- The datasets needed to train NN are typically very large
- Use SGD so that only a small portion of the dataset is needed at a time
  - Each small portion is called a *mini-batch*
  - Use a *momentum* term, which averages the current gradient with those from previous mini-batches.
  - One complete pass through the data is called an *epoch*.

Monitoring training with SGD

- Separate the training set into training and validation
  - use the training set to run backpropagation
  - test the NN on the validation set for diagnostics
    - check for convergence - adjust learning rate if necessary
    - check for diverging loss - adjust learning rate
    - stopping criteria - stop when no change in the validation error.
    - decay learning rate after each epoch.

Load NN software

- We will use *keras*
  - compatible with scikit-learn
  - keras is an easy-to-use front-end for Tensorflow
  - (slides are using Python 3.8 and Tensorflow 2.8)

In [4]:
```
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Activation
from tensorflow.keras import backend as K
import struct
```

In [6]:
```
import sys
print("Python:", sys.version, "Keras:", keras.__version__, "TF:", tf.__version__)
```

```
Python: 3.8.16 (default, Jan 17 2023, 16:39:35)
```

```
[Clang 14.0.6 ] Keras: 2.8.0 TF: 2.8.0
```

- train 1 NN with just one output layer
  - this is the same as logistic regression

In [10]:

```
# clear the session (delete the current NN graph)
K.clear_session()

# initialize random seed
random.seed(4487); tf.random.set_seed(4487)

# convert class labels to class binary vectors (required for Keras)
Yb = keras.utils.to_categorical(Y)

# build the network
nn = Sequential()
nn.add(Dense(units=2,               # number of output nodes (classes)
             input_dim=2,           # input dimension
             activation='softmax' # softmax is for classification
            )
      )
```

```
Metal device set to: Apple M1 Max
```

```
2023-01-22 12:00:07.497101: I tensorflow/core/common_runtime/pluggable_device/plug
gable_device_factory.cc:305] Could not identify NUMA node of platform GPU ID 0, de
faulting to 0. Your kernel may not have been built with NUMA support.
2023-01-22 12:00:07.497245: I tensorflow/core/common_runtime/pluggable_device/plug
gable_device_factory.cc:271] Created TensorFlow device (/job:localhost/replica:0/t
ask:0/device:GPU:0 with 0 MB memory) -> physical PluggableDevice (device: 0, name:
METAL, pci bus id: <undefined>)
```

In [11]:

```
# compile the network
nn.compile(loss=keras.losses.categorical_crossentropy,   # classification loss
     optimizer=keras.optimizers.SGD(  # use SGD for optimization
               learning_rate=0.01,       # learning rate
               momentum=0.9,  # momentum for averaging over batches
               nesterov=True  # use Nestorov momentum
            ))

# fit the network
history = nn.fit(X, Yb,                   # the input/output data
                 epochs=100,              # number of iterations
                 batch_size=32,           # batch size
                 validation_split=0.1, # ratio of data for validation
                 verbose=False            # set to True to see each iteration
                )
```

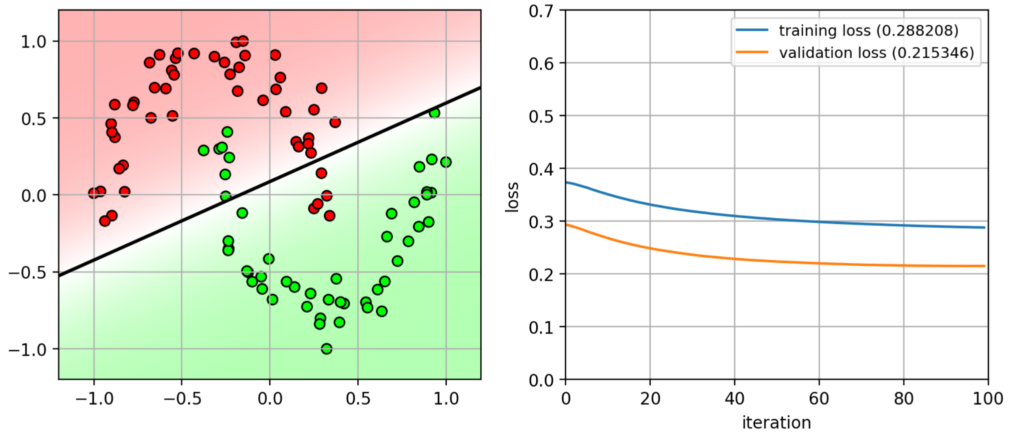
```
2023-01-22 12:00:07.555231: W tensorflow/core/platform/profile_utils/cpu_utils.cc:
128] Failed to get CPU frequency: 0 Hz
2023-01-22 12:00:07.630512: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:00:07.734573: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

- training and validation loss have converged

In [13]:

```
nnfig
```

Out[13]:



- Add one 1 hidden layer with 2 ReLU nodes

In [14]:

```
K.clear_session()
random.seed(5489); tf.random.set_seed(4471) # initialize random seed

# build the network
nn = Sequential()
nn.add(Dense(units=2,                # 2 nodes in the hidden layer
             input_dim=2,
             activation='relu'))
nn.add(Dense(units=2,                # 2 output nodes (one for each class)
             activation='softmax'))

# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
           optimizer=keras.optimizers.SGD(lr=0.3, momentum=0.9, nesterov=True))
history = nn.fit(X, Yb, epochs=100, batch_size=32, validation_split=0.1, verbose=False)
```

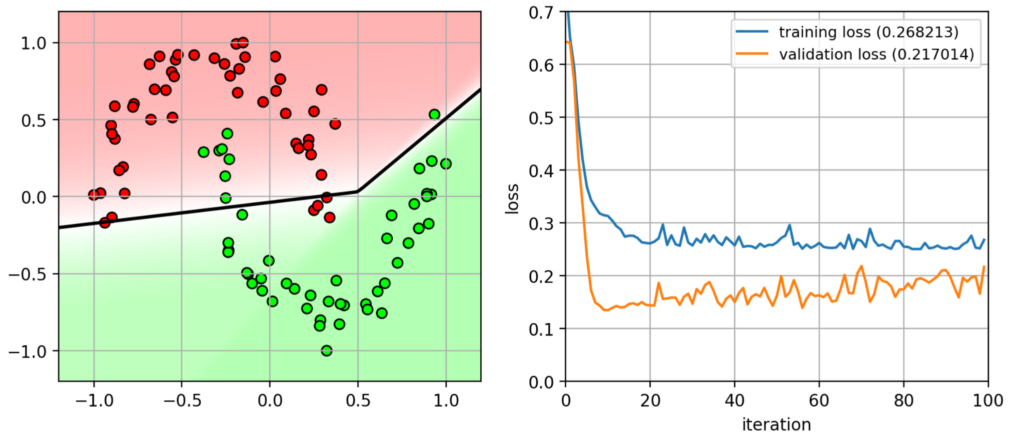
```
/Users/abc/miniforge3/envs/py38tfm28/lib/python3.8/site-packages/keras/optimizer_v
2/gradient_descent.py:102: UserWarning: The `lr` argument is deprecated, use `lear
ning_rate` instead.
  super(SGD, self).__init__(name, **kwargs)
2023-01-22 12:00:12.120748: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:00:12.203370: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

- Add one 1 hidden layer with 2 ReLU nodes
  - can carve out part of the red class.

In [16]:

```
nnfig
```

Out[16]:



- Let's try more nodes
  - 1 hidden layer with 20 hidden nodes

In [17]:

```python
K.clear_session()
random.seed(4487); tf.random.set_seed(4487) # initialize random seed

# build the network
nn = Sequential()
nn.add(Dense(units=20, input_dim=2, activation='relu'))
nn.add(Dense(units=2, activation='softmax'))

# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
    optimizer=keras.optimizers.SGD(lr=0.3, momentum=0.9, nesterov=True))
history = nn.fit(X, Yb, epochs=100, batch_size=32, validation_split=0.1, verbose=False)
```

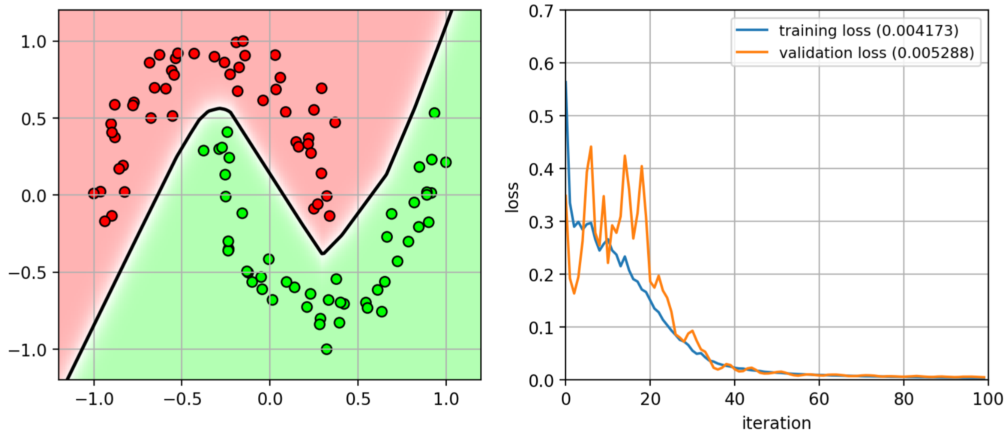
```
2023-01-22 12:00:16.764836: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:00:16.858481: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

- Let's try more nodes
    - 1 hidden layer with 20 hidden nodes
    - with enough nodes, we can get a perfect classifier.

In [19]:

```python
nnfig
```

Out[19]:



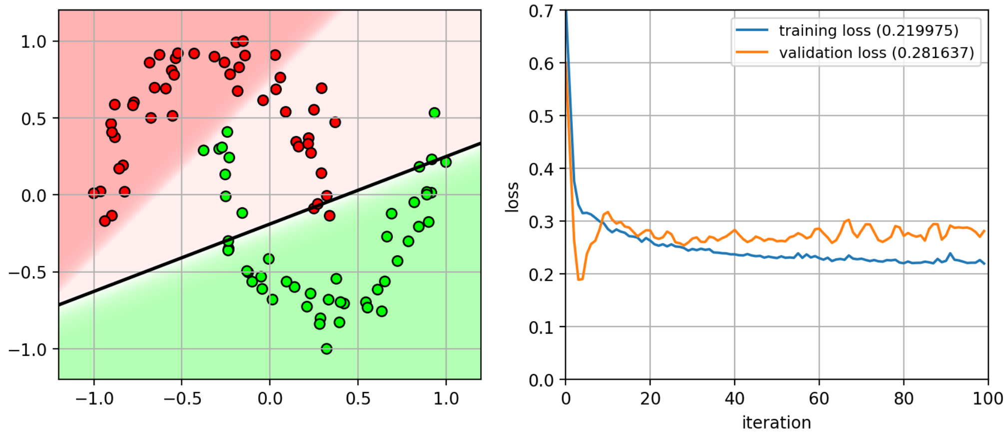
Overfitting

- Continuous training will sometimes lead to overfitting
    - the training loss decreases, but the validation loss increases

In [22]:

```python
nnfig
```

Out[22]:



Early stopping

- Training can be stopped when the validation loss is stable for a number of iterations
  - stable means change below a threshold
  - this is to prevent overfitting the training data.
  - we can limit the number of iterations.
- *We are using the loss/accuracy on the (held-out) validation data to estimate the generalization performance of the network*

In [23]:
```
K.clear_session()
random.seed(248); tf.random.set_seed(3240) # initialize random seed

# build the network
nn = Sequential()
nn.add(Dense(units=2, input_dim=2, activation='relu'))
nn.add(Dense(units=2, activation='softmax'))

# setup early stopping callback function
earlystop = keras.callbacks.EarlyStopping(
    monitor='val_loss',      # look at the validation loss
    min_delta=0.0001,        # threshold to consider as no change
    patience=5,              # stop if 5 epochs with no change
    verbose=1, mode='auto'
)
callbacks_list = [earlystop]

# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
           optimizer=keras.optimizers.SGD(lr=0.3, momentum=0.9, nesterov=True))
history = nn.fit(X, Yb, epochs=100, batch_size=32, validation_split=0.1,
                 verbose=False,
                 callbacks=callbacks_list)  # setup the callback list
```

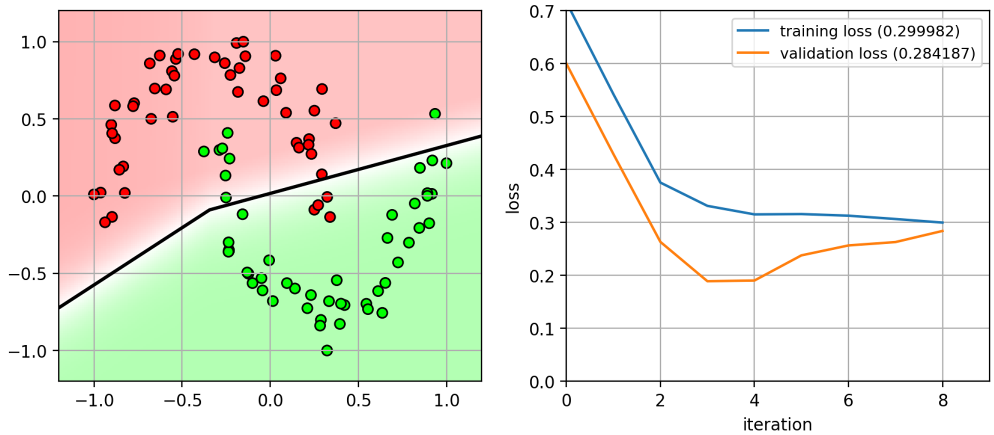
```
2023-01-22 12:00:26.094325: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:00:26.175654: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
Epoch 9: early stopping
```

- training is stopped before overfitting begins.

In [25]:
```
nnfig
```

Out[25]:



Universal Approximation Theorem

- Cybenko (1989), Hornik (1991)
  - *A multi-layer perceptron with a single hidden layer and a finite number of nodes can approximate any continuous function up to a desired error.*
    - The number of nodes needed might be very large.
    - Doesn't say anything about how difficult it is to train it.

- *How many hidden nodes are needed?*
  - In the worst case, consider binary functions mapping $\{0,1\}^n \to \{0,1\}$
    - there are 2^n possible inputs.
    - there are 2^{2^n} possible functions (each input has 2 possible outputs)
    - thus, we need 2^n bits in the hidden layer to select one of these functions.
  - need $O(2^n)$ nodes in the hidden layer, exponential in the size of the input!

- *How to train this model?*
  - According to the "no free lunch theorem", there is no universally best learning algorithm!

- Deep learning corollary
  - *The number of functions representable by a deep network requires an exponential number of nodes for a shallow network with 1 hidden-layer.*
  - A deep network can learn the same function using less nodes.
  - Given the same number of nodes, a deep network can learn more complex functions.
- Doesn't say anything about how difficult it is to train it.

Example

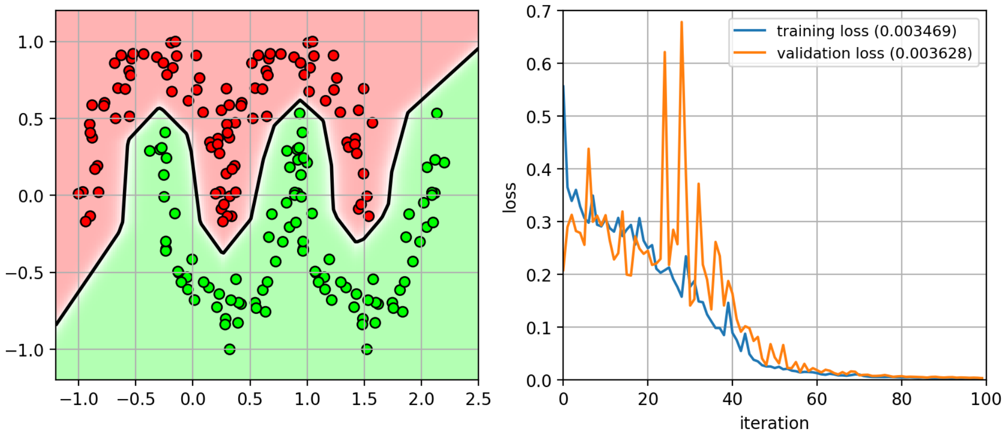
- Network with 1 hidden layer
  - input (2D) -> 40 hidden nodes -> output (2D)

In [29]:
```
nn.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 40)                120

 dense_1 (Dense)             (None, 2)                 82

=================================================================
Total params: 202
Trainable params: 202
Non-trainable params: 0
_________________________________________________________________
```

In [30]:
```
nnfig
```

Out[30]:



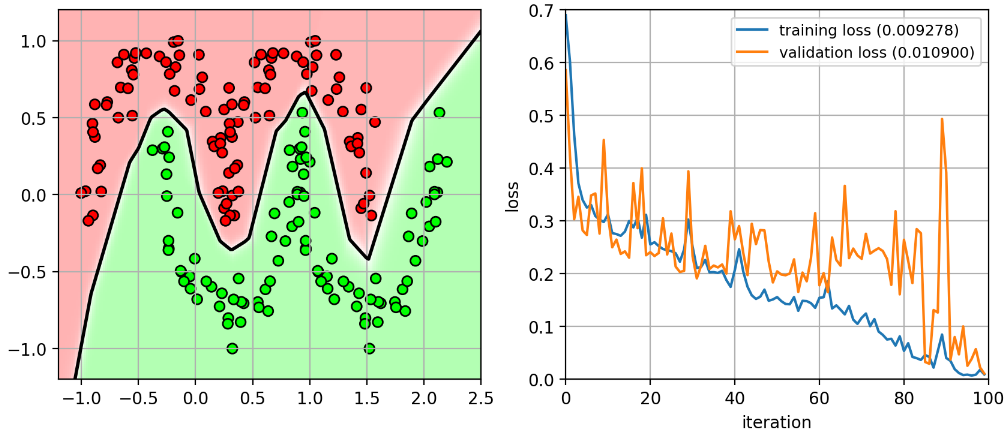
- 3 hidden layers:
  - input (2D) -> 8 nodes -> 5 nodes -> 3 nodes -> output (2D)

In [33]:
```
nn.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 8)                 24

 dense_1 (Dense)             (None, 8)                 72

 dense_2 (Dense)             (None, 3)                 27

 dense_3 (Dense)             (None, 2)                 8

=================================================================
Total params: 131
Trainable params: 131
Non-trainable params: 0
_________________________________________________________________
```

In [34]:
```
nnfig
```

Out[34]:



We should use deeper networks...

- Less parameters than a 1 hidden-layer NN
  - but the number of parameters is still large
- Dataset is still too small.
- *Vanishing Gradient problem*
  - backprop recursively multiplies gradients
    - numerical values get smaller.
    - gradient signal is "washed" out the further back it travels.
- We'll see how to address these problems later.

Example on MNIST Dataset

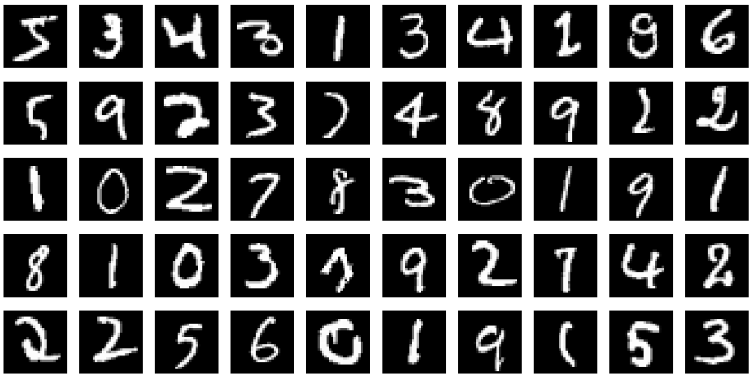
- Images are 28x28, digits 0-9
  - 6,000 for training
  - 10,000 for testing

In [37]:
```
n_train, nrow, ncol, trainimg = read_img('data/train-images.idx3-ubyte')
_, trainY = read_label('data/train-labels.idx1-ubyte')
n_test, _, _, testimg = read_img('data/t10k-images.idx3-ubyte')
_, testY = read_label('data/t10k-labels.idx1-ubyte')

# for demonstration we only use 10% of the training data
sample_index = range(0, trainimg.shape[0], 10)
trainimg  = trainimg[sample_index]
trainY    = trainY[sample_index]
print(trainimg.shape)
print(trainY.shape)
```

```
print(testimg.shape)
print(testY.shape)
```

```
(6000, 28, 28)
(6000,)
(10000, 28, 28)
(10000,)
```

In [38]:
```
# Example images
plt.figure(figsize=(8,4))
show_imgs(trainimg[0:50])
```



Pre-processing

- Reshape images into vectors
- map to [0,1], then subtract the mean

In [39]:
```
# Reshape the images to a vector
# and map the data to [0,1]
trainXraw = trainimg.reshape((len(trainimg), -1), order='C') / 255.0
testXraw = testimg.reshape((len(testimg), -1), order='C') / 255.0

# center the image data (but don't change variance)
scaler = preprocessing.StandardScaler(with_std=False)
trainX = scaler.fit_transform(trainXraw)
testX  = scaler.transform(testXraw)

# convert class labels to binary indicators
trainYb = keras.utils.to_categorical(trainY)

print(trainX.shape)
print(trainYb.shape)
```

```
(6000, 784)
(6000, 10)
```

- Generate a fixed validation set
    - use vtrainX for training and validX for validation

In [40]:
```
# generate a fixed validation set using 10% of the training set
vtrainX, validX, vtrainYb, validYb = \
  model_selection.train_test_split(trainX, trainYb,
  train_size=0.9, test_size=0.1, random_state=4487)

# validation data
validset  = (validX, validYb)
```

MNIST - Logistic Regression (0-hidden layers)

- Training procedure

- We specify the validation set so that it will be fixed when we change the `random_state` to randomly initialize the weights.
- Train on the non-validation training data

In [42]:
```
K.clear_session()  # cleanup
random.seed(4487); tf.random.set_seed(4487) # initialize seed

# build the network
nn = Sequential()
nn.add(Dense(units=10, input_dim=784, activation='softmax'))

# early stopping criteria
earlystop = keras.callbacks.EarlyStopping(
               monitor='val_accuracy',     # use validation accuracy for stopping
                                           # (use 'val_acc' for tf1)
               min_delta=0.0001, patience=5,
               verbose=1, mode='auto')
callbacks_list = [earlystop]

# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
           optimizer=keras.optimizers.SGD(learning_rate=0.05, momentum=0.9, nesterov=True),
           metrics=['accuracy']  # also calculate accuracy during training
          )

history = nn.fit(vtrainX, vtrainYb, epochs=100, batch_size=50,
                 callbacks=callbacks_list,
                 validation_data=validset,  # specify the validation set
                 verbose=False)
```

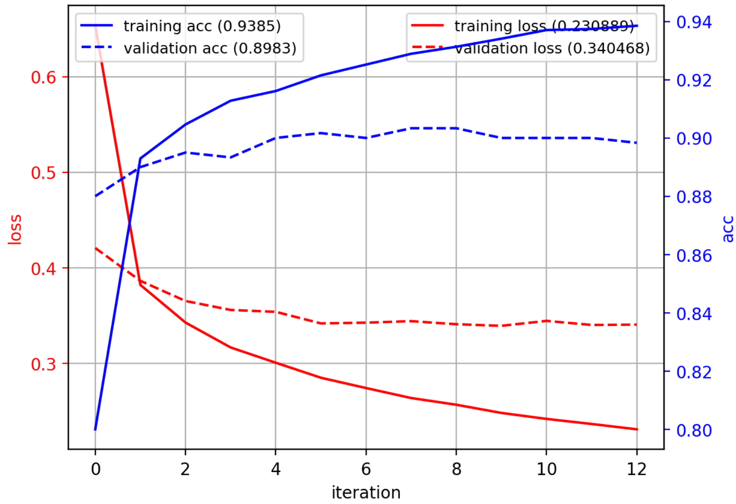
```
2023-01-22 12:00:41.827037: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:00:42.355215: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
Epoch 13: early stopping
```

In [43]:
```
plot_history(history)

predY = argmax(nn.predict(testX, verbose=False), axis=-1)
acc = metrics.accuracy_score(testY, predY)
print("test accuracy:", acc)
```

```
2023-01-22 12:00:48.813260: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
test accuracy: 0.8911
```



- Examine the weights of the network
  - use `get_layer` to access indexed layer in the network
    - layer 0 is the input layer.
  - use `get_weights` to get the weights/biases for a layer.

In [44]:
```
nn.summary()
```

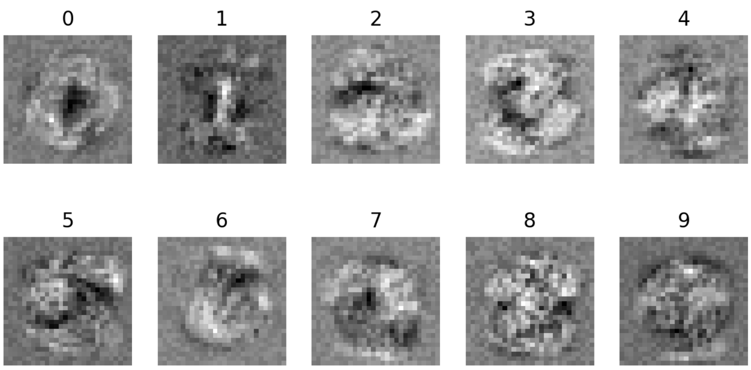
```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #   
=================================================================
 dense (Dense)               (None, 10)                7850      
                                                                 
=================================================================
Total params: 7,850
Trainable params: 7,850
Non-trainable params: 0
_________________________________________________________________
```

In [45]:
```
params = nn.get_layer(index=0).get_weights()
print(params)
```

```
[array([[-0.07668316,  0.0506426 ,  0.02011225, ..., -0.06035375,
        -0.02619639, -0.04660042],
       [ 0.02124737, -0.03975144, -0.0652017 , ...,  0.02619619,
         0.00104643,  0.07461943],
       [-0.00434513, -0.05478361,  0.08619549, ..., -0.02323265,
         0.01046359,  0.02967306],
       ...,
       [ 0.00080693, -0.07145306,  0.08062453, ...,  0.01938874,
        -0.06666604, -0.06500553],
       [ 0.01731288,  0.00918476,  0.0270523 , ..., -0.02666005,
         0.04110996,  0.02432326],
       [-0.08605715,  0.06289775,  0.0517082 , ...,  0.06466276,
        -0.08470873,  0.041274  ]], dtype=float32), array([-1.1132437 , -1.4380776
,  0.5278839 ,  0.53613126, -0.73726153,
        0.9060908 , -0.6181745 , -0.5193604 ,  1.6782092 ,  0.7777992 ],
      dtype=float32)]
```

- Reshape the weights into an image
  - input images that match the weights will have high response for that class.

In [46]:
```
W = params[0]
filter_list = [W[:,i].reshape((28,28)) for i in range(W.shape[1])]
plt.figure(figsize=(8,4))
show_imgs(filter_list, nc=5, titles="%d")
```



MNIST - 1-hidden layer

- Add 1 hidden layer with 50 ReLu nodes
  - each node is extracting a feature from the input image

In [47]:
```
K.clear_session()  # cleanup
random.seed(4487); tf.random.set_seed(4487) # initialize seed

# build the network
nn = Sequential()
nn.add(Dense(units=50, input_dim=784, activation='relu')) # hidden layer
nn.add(Dense(units=10, activation='softmax'))  # output layer
```

```python
# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
           optimizer=keras.optimizers.SGD(learning_rate=0.1, momentum=0.9, nesterov=True),
           metrics=['accuracy'])
history = nn.fit(vtrainX, vtrainYb, epochs=100, batch_size=50,
                 callbacks=callbacks_list,
                 validation_data=validset, verbose=False)
```

```
2023-01-22 12:00:49.612988: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:00:50.199928: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
Epoch 10: early stopping
```

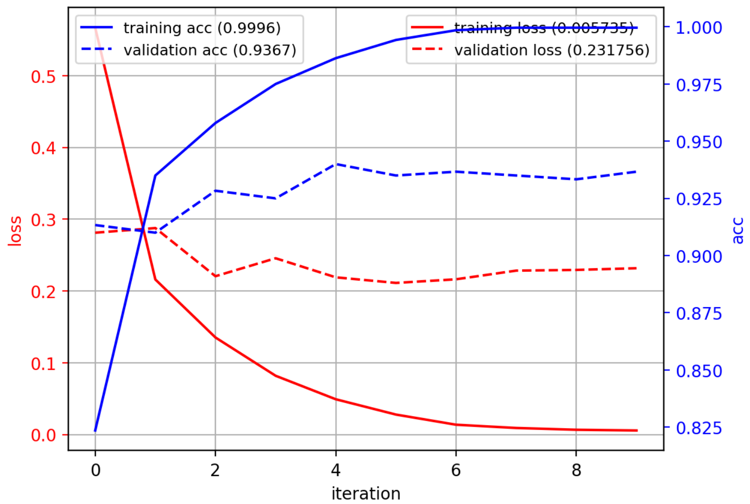
In [48]:
```python
nn.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 50)                39250

 dense_1 (Dense)             (None, 10)                510

=================================================================
Total params: 39,760
Trainable params: 39,760
Non-trainable params: 0
_________________________________________________________________
```

In [49]:
```python
plot_history(history)

predY = argmax(nn.predict(testX, verbose=False), axis=-1)
acc = metrics.accuracy_score(testY, predY)
print("test accuracy:", acc)
```

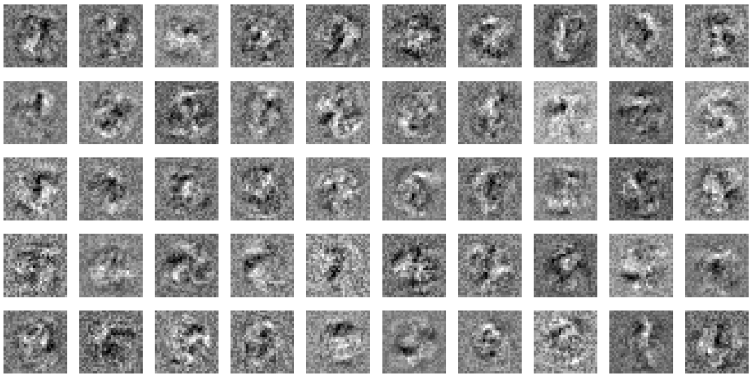
```
2023-01-22 12:00:55.495294: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
test accuracy: 0.938
```



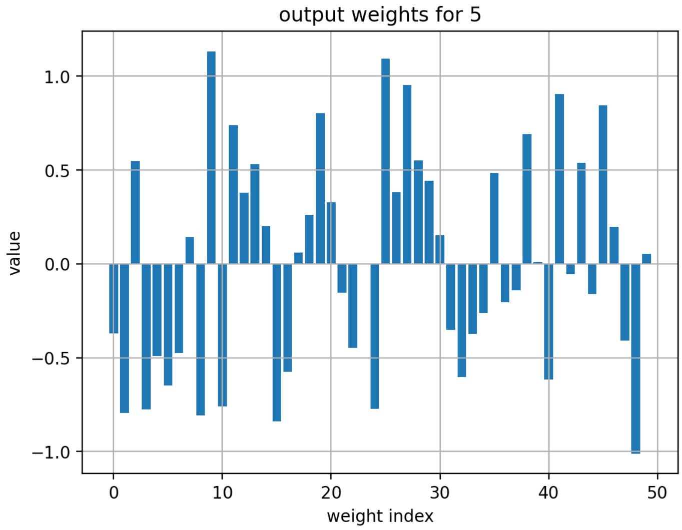
- Examine the weights of the hidden layer
  - $h_i = \sigma(\mathbf{w}_i^T \mathbf{x})$
  - each weight vector is a "pattern prototype" that the node will match
- The hidden nodes look for local structures:
  - oriented edges, curves, other local structures

In [50]:
```python
W = nn.get_layer(index=0).get_weights()[0]
filter_list = [W[:,i].reshape((28,28)) for i in range(W.shape[1])]
```



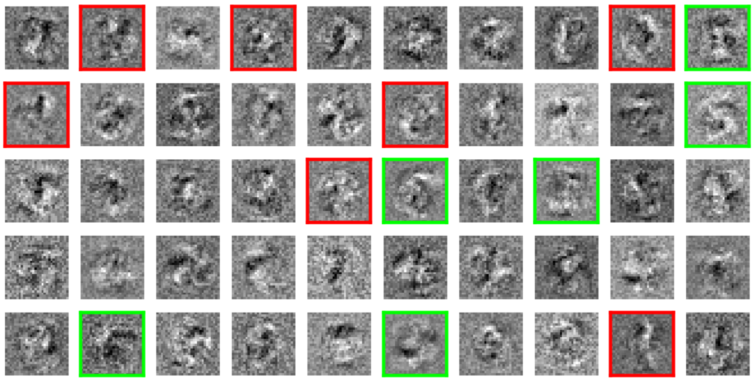
- Examine the weights of the 2nd layer (output)
  - $y_j = \sigma(\mathbf{w}_j^T \mathbf{h})$
  - recall the hidden-layer outputs h are always non-negative.
    - positive value in $\mathbf{w}_j \rightarrow$ class j should have j-th pattern
    - negative value in $\mathbf{w}_j \rightarrow$ class j shouldn't have j-th pattern

In [51]:
```
W = nn.get_layer(index=1).get_weights()[0]
d = 5
plt.bar(arange(0,W.shape[0]),W[:,d]); plt.grid(True);
plt.xlabel('weight index'); plt.ylabel('value')
plt.title('output weights for {}'.format(d));
```



- For "5", finds local image parts that correspond to 5
  - should have (green boxes):
    - horizontal line at top; semicircle on the bottom
  - shouldn't have (red boxes):
    - verticle line in top-right; verticle line in the middle

In [52]:
```
plt.figure(figsize=(8,4))
show_imgs(filter_list, nc=10,
          highlight_green=(W[:,d]>0.75), # positive weights are green
          highlight_red=(W[:,d]<-0.75))  # negative weights are red
```



1 Hidden layer with more nodes

- hidden layer with 200 nodes

In [53]:
```
K.clear_session()  # cleanup
random.seed(4487); tf.random.set_seed(4487)  # initialize seed

# build the network
nn = Sequential()
nn.add(Dense(units=200, input_dim=784, activation='relu'))
nn.add(Dense(units=10, activation='softmax'))

# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
           optimizer=keras.optimizers.SGD(learning_rate=0.1, momentum=0.9, nesterov=True),
           metrics=['accuracy'])
history = nn.fit(vtrainX, vtrainYb, epochs=100, batch_size=50,
                 callbacks=callbacks_list,
                 validation_data=validset, verbose=False)
```

```
2023-01-22 12:00:57.214617: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:00:57.812820: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
Epoch 8: early stopping
```

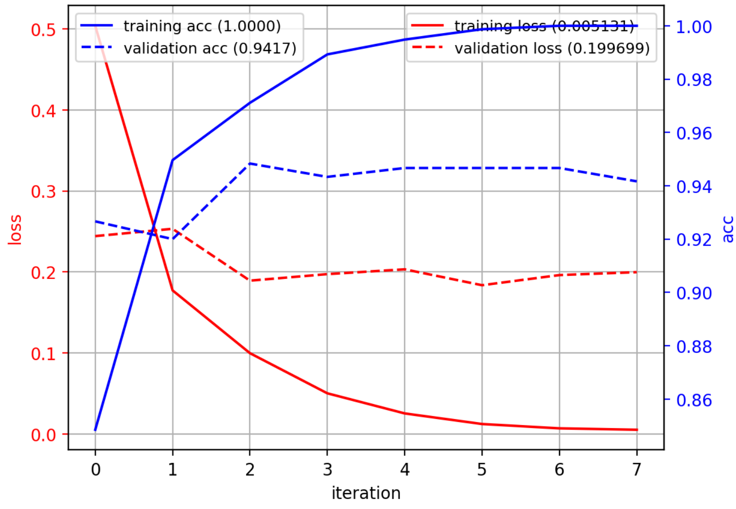
In [54]:
```
nn.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 200)               157000

 dense_1 (Dense)             (None, 10)                2010

=================================================================
Total params: 159,010
Trainable params: 159,010
Non-trainable params: 0
_________________________________________________________________
```

In [55]:
```
plot_history(history)
predY = argmax(nn.predict(testX, verbose=False), axis=-1)
acc = metrics.accuracy_score(testY, predY)
print("test accuracy: ", acc)
```

```
2023-01-22 12:01:01.966204: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
test accuracy:  0.9437
```



- hidden layer with 1000 nodes

In [56]:
```
K.clear_session()  # cleanup
random.seed(4487); tf.random.set_seed(4487)  # initialize seed

# build the network
nn = Sequential()
nn.add(Dense(units=1000, input_dim=784, activation='relu'))
nn.add(Dense(units=10, activation='softmax'))

# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
           optimizer=keras.optimizers.SGD(learning_rate=0.1, momentum=0.9, nesterov=True),
          metrics=['accuracy'])
history = nn.fit(vtrainX, vtrainYb, epochs=100, batch_size=50,
                 callbacks=callbacks_list,
                 validation_data=validset, verbose=False)
```

```
2023-01-22 12:01:02.697350: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:01:03.305985: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
Epoch 8: early stopping
```

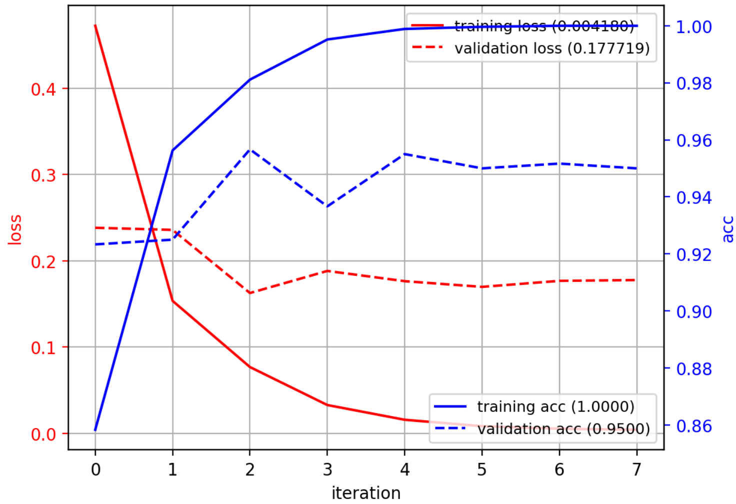
In [57]:
```
nn.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 1000)              785000

 dense_1 (Dense)             (None, 10)                10010

=================================================================
Total params: 795,010
Trainable params: 795,010
Non-trainable params: 0
_________________________________________________________________
```

In [58]:
```
plot_history(history)
predY = argmax(nn.predict(testX, verbose=False), axis=-1)
acc = metrics.accuracy_score(testY, predY)
print("test accuracy:", acc)
```

```
2023-01-22 12:01:07.619910: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
test accuracy: 0.9462
```



- 2 hidden layers
  - input (28x28) -> 500 nodes -> 500 nodes -> output
  - Slightly better

In [59]:
```
K.clear_session()  # cleanup
random.seed(4487); tf.random.set_seed(4487)  # initialize seed

# build the network
nn = Sequential()
nn.add(Dense(units=500, input_dim=784, activation='relu'))
nn.add(Dense(units=500, activation='relu'))
nn.add(Dense(units=10, activation='softmax'))

# compile and fit the network
nn.compile(loss=keras.losses.categorical_crossentropy,
           optimizer=keras.optimizers.SGD(learning_rate=0.1, momentum=0.9, nesterov=True),
          metrics=['accuracy'])
history = nn.fit(vtrainX, vtrainYb, epochs=100, batch_size=50,
                 callbacks=callbacks_list,
                 validation_data=validset, verbose=False)
```

```
2023-01-22 12:01:08.297196: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
2023-01-22 12:01:08.939766: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
Epoch 12: early stopping
```

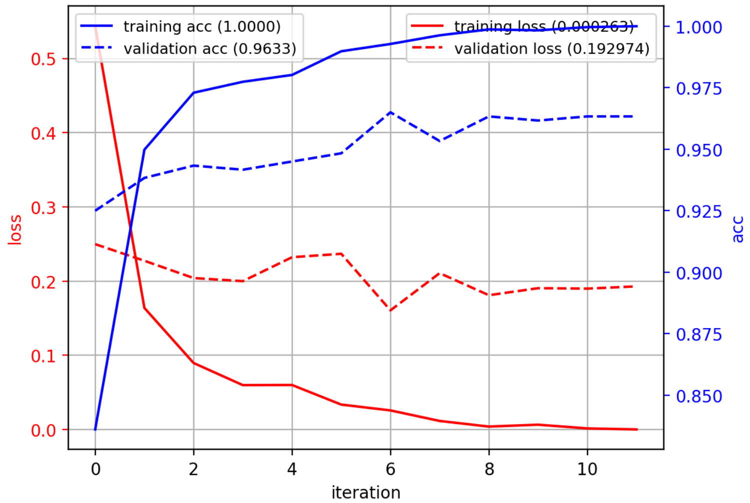
In [60]:
```
nn.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 500)               392500

 dense_1 (Dense)             (None, 500)               250500

 dense_2 (Dense)             (None, 10)                5010

=================================================================
Total params: 648,010
Trainable params: 648,010
Non-trainable params: 0
_________________________________________________________________
```

In [61]:
```
plot_history(history)
predY = argmax(nn.predict(testX, verbose=False), axis=-1)
acc = metrics.accuracy_score(testY, predY)
print("test accuracy:", acc)
```

```
2023-01-22 12:01:16.538321: I tensorflow/core/grappler/optimizers/custom_graph_opt
imizer_registry.cc:113] Plugin optimizer for device_type GPU is enabled.
```

```
test accuracy: 0.9529
```



Comparison on MNIST

- Performance is saturated.

Type	No.Layers	Architecture	No.Parameters	Test Accuracy
LR	1	output(10)	7,850	0.8911
MLP	2	ReLu(50), output(10)	39,760	0.9380
MLP	2	Relu(200), output(10)	159,010	0.9437
MLP	2	Relu(1000), output(10)	795,010	0.9462
MLP	3	ReLu(500), Relu(500), output(10)	648,010	0.9529

Summary

- **Different types of neural networks**
  - *Perceptron* - single node (similar to logistic regression)
  - *Multi-layer perceptron (MLP)* - collection of perceptrons in layers
    - also called *fully-connected layers* or *dense layers*
- **Training**
  - optimize loss function using stochastic gradient descent

- **Advantages**
  - lots of parameters - large capacity to learn from large amounts of data
- **Disadvantages**
  - lots of parameters - easy to overfit data
    - need to monitor the training process
  - sensitive to initialization, learning rate, training algorithm.

Other things

- **Numerical stability**
  - normalize the inputs to [-1,1] or [0,1]
- **Improving speed**
  - parallelize computations using GPU (Nvidia+CUDA)
- **Initialization**
  - the resulting network is still sensitive to initialization.

        - Solution: train several networks and combine them as an ensemble.
- **Training problems**
    - For very deep networks, the "vanishing gradient" problem can hinder convergence
    - lack of data
    - We will see how to address these problems later.

References

- Software

    - Tensorflow (Google)- https://www.tensorflow.org
    - Keras - https://keras.io
        - Easy-to-use front-end for deep learning
        - Included with tensorflow
        - API Documentation: https://keras.io/layers/core/
    - see Canvas site for installation tips.
- History:

    - http://www.andreykurenkov.com/writing/a-brief-history-of-neural-nets-and-deep-learning/
- Keras tutorials:

    - https://elitedatascience.com/keras-tutorial-deep-learning-in-python
    - https://blog.keras.io
- Online courses::

    - http://cs231n.github.io/neural-networks-1/
    - http://cs231n.github.io/convolutional-networks/