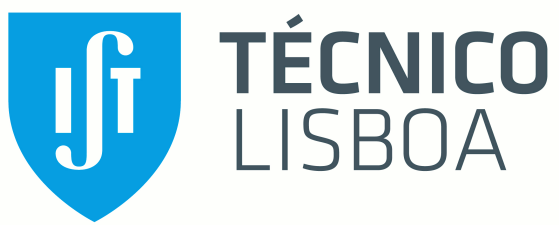
Lecture 5: Neural Networks II

André Martins, Francisco Melo, Mário Figueiredo



Deep Learning Course, Winter 2022-2023

Today's Roadmap

Last lecture was about neural networks:

- From perceptron to multi-layer perceptron
- Feed-forward neural networks
- Activation funcions: sigmoid, tanh, relu, ...
- Activation maps: softmax, sparsemax, ...
- Non-convex optimization and local minima
- Universal approximation theorem
- Gradient backpropagation

Today: autodiff, regularization, tricks of the trade.

Outline

Outline

Recap: Forward Propagation

Now assume $L \geq 1$ hidden layers:

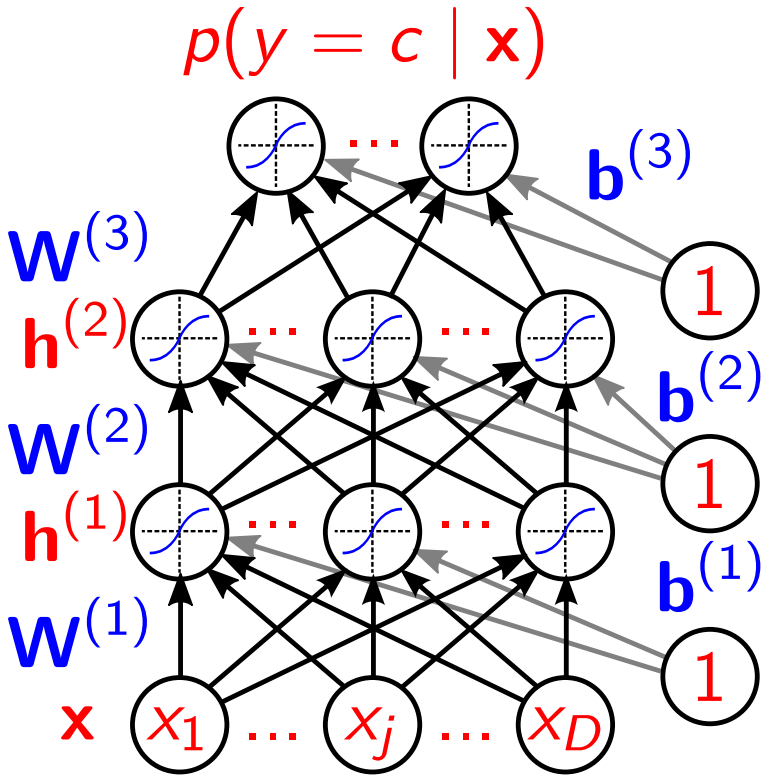
- **Hidden layer pre-activation** (define $\boldsymbol{h}^{(0)} = \boldsymbol{x}$, for convenience):

$$\boldsymbol{z}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{W}^{(\ell)} \boldsymbol{h}^{(\ell-1)}(\boldsymbol{x}) + \boldsymbol{b}^{(1)},$$

  with $\boldsymbol{W}^{(\ell)} \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$ and $\boldsymbol{b}^{(\ell)} \in \mathbb{R}^{K_\ell}$.

- **Hidden layer activation:**

$$\boldsymbol{h}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{z}^{(\ell)}(\boldsymbol{x})).$$



- **Output layer activation:**

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{o}(\boldsymbol{z}^{(L+1)}(\boldsymbol{x})) = \boldsymbol{o}(\boldsymbol{W}^{(L+1)} \boldsymbol{h}^{(L)} + \boldsymbol{b}^{(L+1)}).$$

Recap: Gradient Backpropagation

Compute output gradient (before activation):

$$\nabla_{\boldsymbol{z}^{(L+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = -(1_y - \boldsymbol{f}(\boldsymbol{x}))$$

for ℓ from $L+1$ to 1 **do**

Compute gradients of hidden layer parameters:

$$\begin{aligned} \nabla_{\boldsymbol{W}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) &= \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)\ \boldsymbol{h}^{(\ell-1)\top} \\ \nabla_{\boldsymbol{b}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) &= \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \end{aligned}$$

Compute gradient of previous hidden layer:

$$\nabla_{\boldsymbol{h}^{(\ell-1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \boldsymbol{W}^{(\ell)\top} \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$$

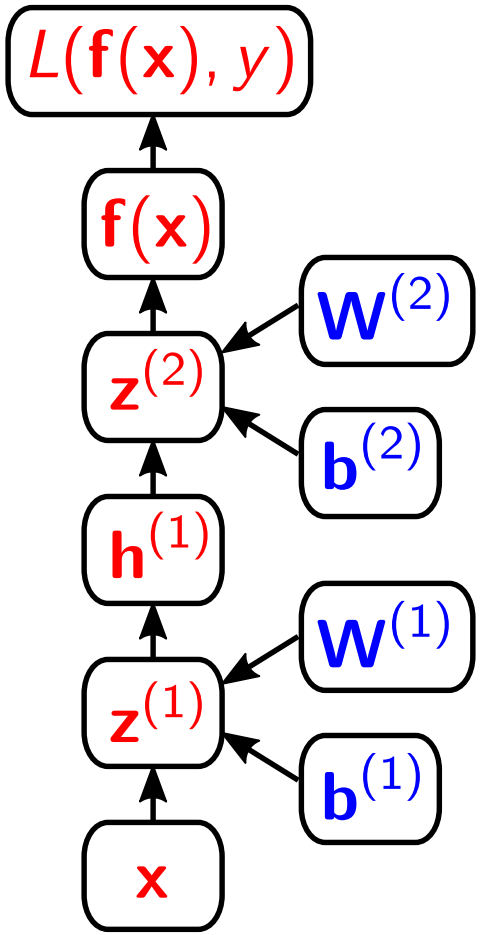
Compute gradient of previous hidden layer (before activation):

$$\nabla_{\boldsymbol{z}^{(\ell-1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{h}^{(\ell-1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \odot \boldsymbol{g}'(\boldsymbol{z}^{(\ell-1)})$$

end for

Computation Graph

- Forward propagation can be represented as a DAG (directed acyclic graph).



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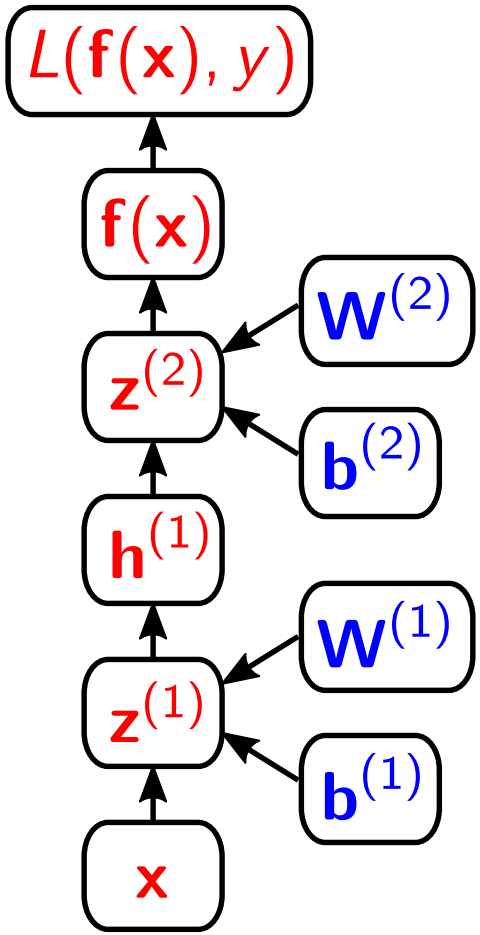

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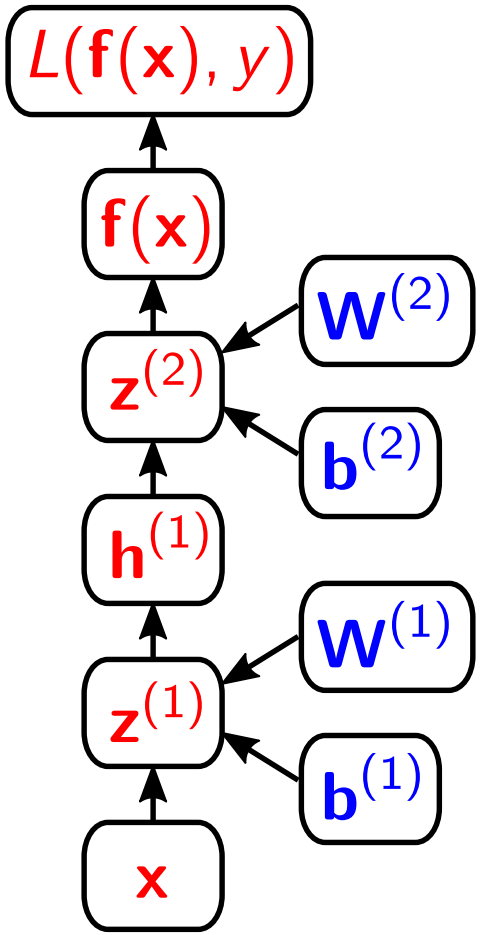
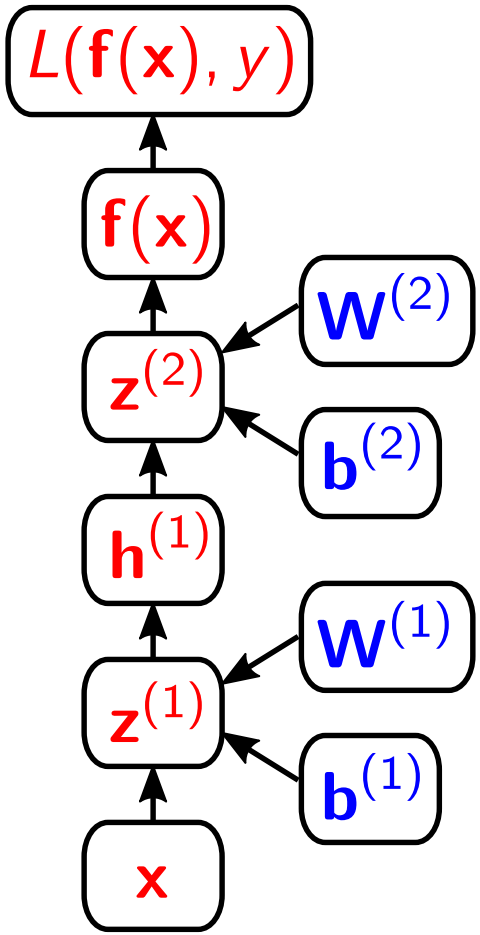


Computation Graph

- Forward propagation can be represented as a DAG (directed acyclic graph).
- Allows implementing forward propagation in a modular way.
- Each box can be an object with a `fprop` method, which computes the output of the box given its inputs.
- Calling the `fprop` method of each box in the right order yields forward propagation.



Automatic Differentiation (Autodiff)

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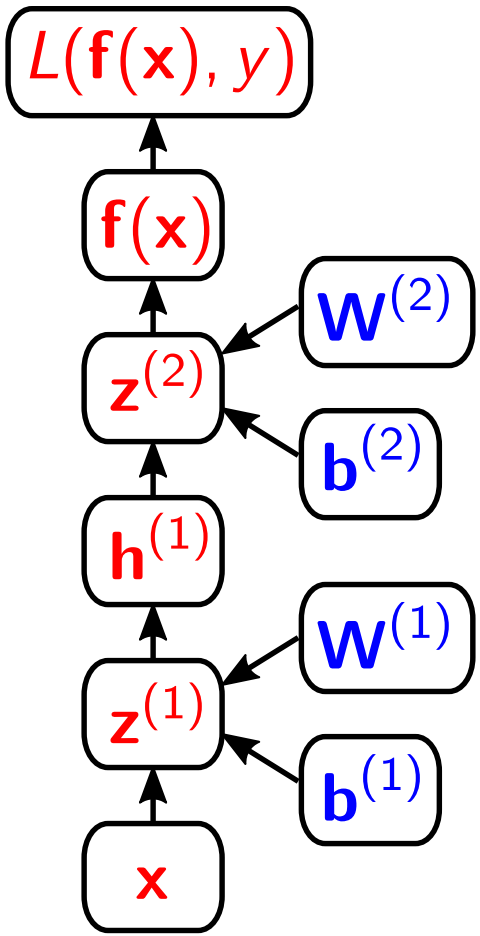

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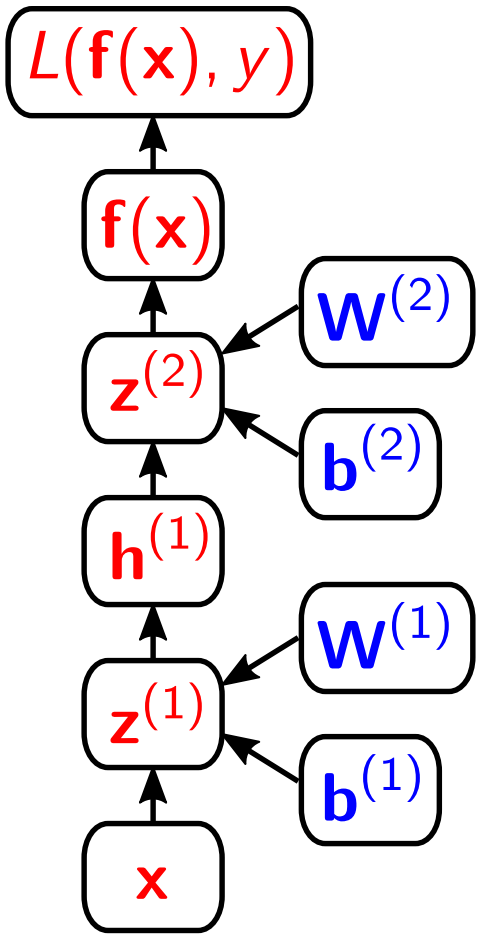
- Each box should have a `bprop` method, which computes the loss gradient w.r.t. its parents, given the loss gradient w.r.t. to the output.



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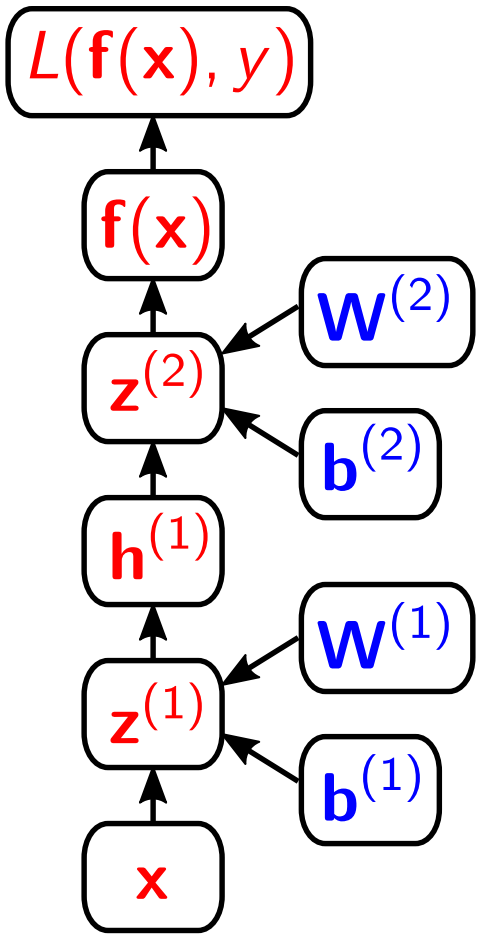

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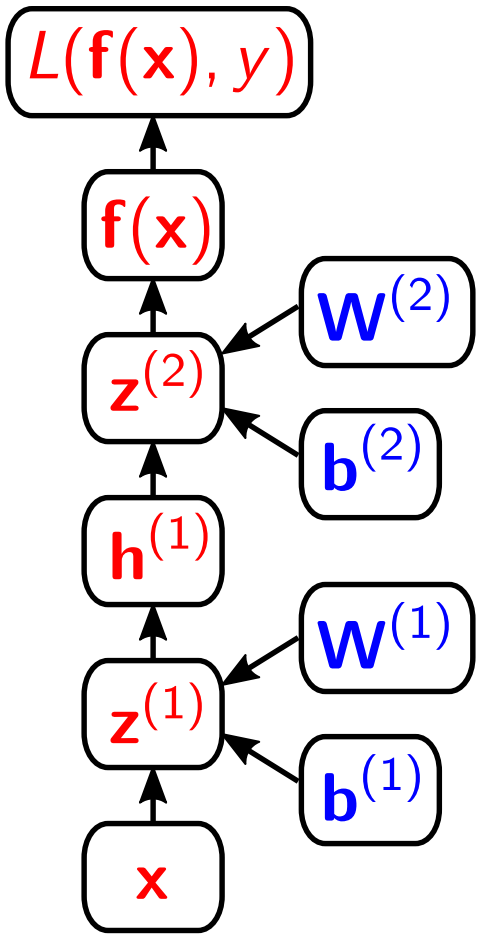
- Each box should have a `bprop` method, which computes the loss gradient w.r.t. its parents, given the loss gradient w.r.t. to the output.
- Can make use of cached computation done during the `fprop` method
- Calling the `bprop` method in reverse order yields backpropagation
  (only needs to reach the parameters)



Several Autodiff Strategies

Symbol-to-number differentiation (Caffe, Torch, Pytorch, Dynet, ...)

- Take a computational graph and numerical inputs, returns a set of numerical values describing the gradient at those input values.
- Advantage: simpler to implement and debug.
- Disadvantage: only works for first-order derivatives.

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Symbol-to-symbol differentiation (Theano, Tensorflow, ...)

- Take a computational graph and add additional nodes to the graph that provide a symbolic description of the desired derivatives (i.e. the derivatives are just another computational graph)
- Advantage: generalizes automatically to higher-order derivatives
- Disadvantage: harder to implement and to debug

Many Software Toolkits for Neural Networks

- Theano
- Tensorflow
- Torch, Pytorch
- MXNet
- Keras
- Caffe
- DyNet
- ...

All implement automatic differentiation.

Some Theano Code (Logistic Regression)

```
import numpy
import theano
import theano.tensor as T
rng = numpy.random

N = 400                                   # training sample size
feats = 784                               # number of input variables

# generate a dataset: D = (input_values, target_class)
D = (rng.randn(N, feats), rng.randint(size=N, low=0, high=2))
training_steps = 10000

# Declare Theano symbolic variables
x = T.dmatrix("x")
y = T.dvector("y")

# initialize the weight vector w randomly
#
# this and the following bias variable b
# are shared so they keep their values
# between training iterations (updates)
w = theano.shared(rng.randn(feats), name="w")

# initialize the bias term
b = theano.shared(0., name="b")

print("Initial model:")
print(w.get_value())
print(b.get_value())

# Construct Theano expression graph
p_1 = 1 / (1 + T.exp(-T.dot(x, w) - b))   # Probability that target = 1
prediction = p_1 > 0.5                    # The prediction thresholded
xent = -y * T.log(p_1) - (1-y) * T.log(1-p_1) # Cross-entropy loss function
cost = xent.mean() + 0.01 * (w ** 2).sum()# The cost to minimize
gw, gb = T.grad(cost, [w, b])             # Compute the gradient of the cost
                                          # w.r.t weight vector w and
                                          # bias term b
                                          # (we shall return to this in a
                                          # following section of this tutorial)

# Compile
train = theano.function(
          inputs=[x,y],
```

Some Code in Tensorflow (Linear Regression)

```
import tensorflow as tf
import numpy as np

# Create 100 phony x, y data points in NumPy, y = x * 0.1 + 0.3
x_data = np.random.rand(100).astype(np.float32)
y_data = x_data * 0.1 + 0.3

# Try to find values for W and b that compute y_data = W * x_data + b
# (We know that W should be 0.1 and b 0.3, but TensorFlow will
# figure that out for us.)
W = tf.Variable(tf.random_uniform([1], -1.0, 1.0))
b = tf.Variable(tf.zeros([1]))
y = W * x_data + b

# Minimize the mean squared errors.
loss = tf.reduce_mean(tf.square(y - y_data))
optimizer = tf.train.GradientDescentOptimizer(0.5)
train = optimizer.minimize(loss)

# Before starting, initialize the variables.  We will 'run' this first.
init = tf.global_variables_initializer()

# Launch the graph.
sess = tf.Session()
sess.run(init)

# Fit the line.
for step in range(201):
    sess.run(train)
    if step % 20 == 0:
        print(step, sess.run(W), sess.run(b))

# Learns best fit is W: [0.1], b: [0.3]
```

Some Code in Keras (Multi-Layer Perceptron)

Multilayer Perceptron (MLP) for multi-class softmax classification:

```
from keras.models import Sequential
from keras.layers import Dense, Dropout, Activation
from keras.optimizers import SGD

model = Sequential()
# Dense(64) is a fully-connected layer with 64 hidden units.
# in the first layer, you must specify the expected input data shape:
# here, 20-dimensional vectors.
model.add(Dense(64, input_dim=20, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(64, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(10, init='uniform'))
model.add(Activation('softmax'))

sgd = SGD(lr=0.1, decay=1e-6, momentum=0.9, nesterov=True)
model.compile(loss='categorical_crossentropy',
              optimizer=sgd,
              metrics=['accuracy'])

model.fit(X_train, y_train,
          nb_epoch=20,
          batch_size=16)
score = model.evaluate(X_test, y_test, batch_size=16)
```

Some Code in Pytorch (Multi-Layer Perceptron)

```
# Fully connected neural network with one hidden layer
class NeuralNet(nn.Module):
    def __init__(self, input_size, hidden_size, num_classes):
        super(NeuralNet, self).__init__()
        self.fc1 = nn.Linear(input_size, hidden_size)
        self.relu = nn.ReLU()
        self.fc2 = nn.Linear(hidden_size, num_classes)

    def forward(self, x):
        out = self.fc1(x)
        out = self.relu(out)
        out = self.fc2(out)
        return out

model = NeuralNet(input_size, hidden_size, num_classes).to(device)

# Loss and optimizer
criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

# Train the model
total_step = len(train_loader)
for epoch in range(num_epochs):
    for i, (images, labels) in enumerate(train_loader):
        # Move tensors to the configured device
        images = images.reshape(-1, 28*28).to(device)
        labels = labels.to(device)

        # Forward pass
        outputs = model(images)
        loss = criterion(outputs, labels)

        # Backward and optimize
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if (i+1) % 100 == 0:
            print ('Epoch [{}/{}], Step [{}/{}], Loss: {:.4f}'
                   .format(epoch+1, num_epochs, i+1, total_step, loss.item()))
```

Reminder: Key Ingredients of SGD

In sum, we need the following ingredients:

- The loss function $L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$ ✓
- A procedure for computing the gradients $\nabla_{\boldsymbol{\theta}} L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$ ✓
- The regularizer $\Omega(\boldsymbol{\theta})$ and its gradient: next!

Outline

Regularization

Recall that we're minimizing the following objective function:

$$\mathcal{L}(\boldsymbol{\theta}) := \lambda\Omega(\boldsymbol{\theta}) + \frac{1}{N}\sum_{n=1}^{N} L(\boldsymbol{f}(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i)$$

It remains to define the regularizer and its gradient

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We will study:

- ℓ_2 regularization
- ℓ_1 regularization
- dropout regularization

ℓ_2 Regularization

- The biases $\boldsymbol{b}^{(1)}, ..., \boldsymbol{b}^{(L+1)}$ are not regularized; only the weights:

$$\Omega(\boldsymbol{\theta}) = \frac{1}{2} \sum_{\ell=1}^{L+1} \|\boldsymbol{W}^{(\ell)}\|^2$$

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- Weight decay effect (as seen in the previous lecture)

$$\begin{aligned} \boldsymbol{W}^{(\ell)} &\leftarrow \boldsymbol{W}^{(\ell)} - \eta \nabla_{\boldsymbol{W}^{(\ell)}} \mathcal{L}_i(\boldsymbol{\theta}) \\ &= \boldsymbol{W}^{(\ell)} - \eta (\lambda \nabla_{\boldsymbol{W}^{(\ell)}} \Omega(\boldsymbol{\theta}) + \nabla_{\boldsymbol{W}^{(\ell)}} L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)) \\ &= \underbrace{(1 - \eta\lambda)}_{<1} \boldsymbol{W}^{(\ell)} - \eta \nabla_{\boldsymbol{W}^{(\ell)}} L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i) \end{aligned}$$

ℓ_1 Regularization

- The biases $\boldsymbol{b}^{(1)}, ..., \boldsymbol{b}^{(L+1)}$ are not regularized; only the weights:

$$\Omega(\boldsymbol{\theta}) = \sum_{\ell} \|\boldsymbol{W}^{(\ell)}\|_1 = \sum_{\ell} \sum_{ij} |W_{ij}^{(\ell)}|$$

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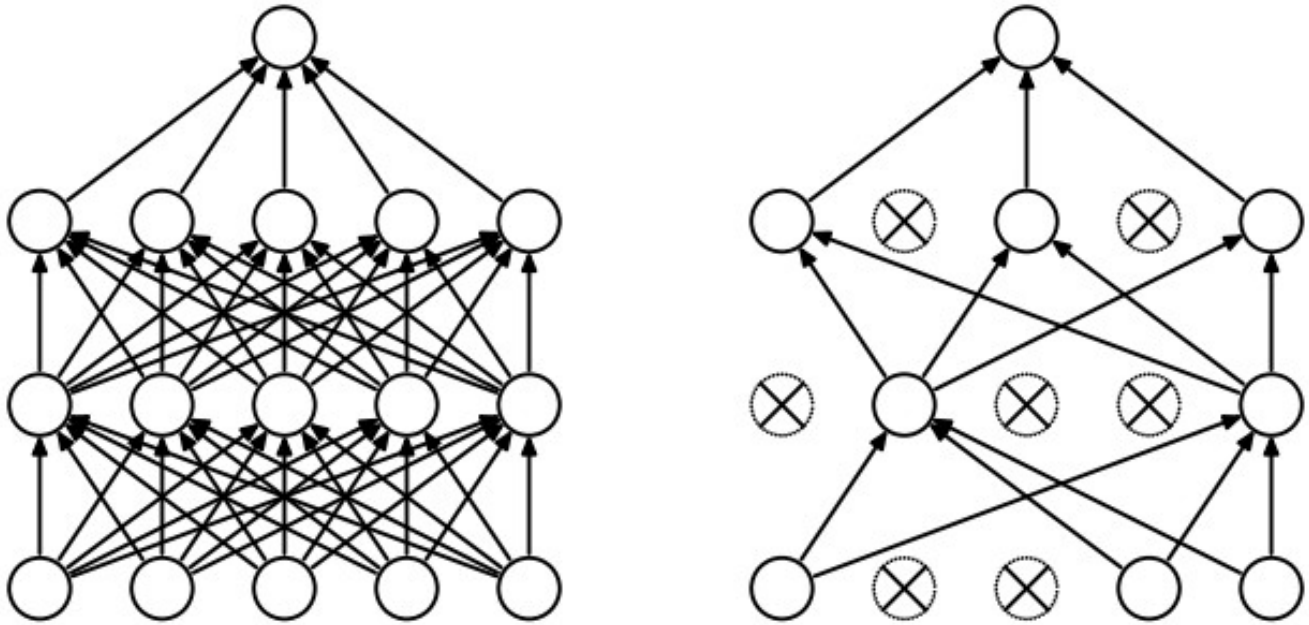
- Equivalent to Laplacian prior on the weights
- Gradient is: $\nabla_{\boldsymbol{W}^{(\ell)}} \Omega(\boldsymbol{\theta}) = \text{sign}(\boldsymbol{W}^{(\ell)})$
- Promotes sparsity of the weights

Dropout Regularization (Srivastava et al., 2014)



(a) Standard Neural Net

(b) After applying dropout.

During training, remove some hidden units, chosen at random

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- At test time, keep all units, with the outputs multiplied by $1 - p$
- Shown to be a form of adaptive regularization (Wager et al., 2013)
- Many software packages implement another variant, inverted dropout, where at training time the output of the units that were not dropped is divided by $1 - p$ and requires no change at test time

Implementation of Dropout

- Usually implemented using random binary masks

- The hidden layer activations become

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- Beats regular backpropagation on many datasets (Hinton et al., 2012)
- Other variants, e.g. DropConnect (Wan et al., 2013), Stochastic Pooling (Zeiler and Fergus, 2013)

Backpropagation with Dropout

Compute output gradient (before activation):

$$\nabla_{\boldsymbol{z}^{(L+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = -(1_y - \boldsymbol{f}(\boldsymbol{x}))$$

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Compute gradients of hidden layer parameters:

$$\nabla_{\boldsymbol{W}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \underbrace{\boldsymbol{h}^{(\ell-1)\top}}_{\text{includes } \boldsymbol{m}^{(\ell-1)}}$$

$$\nabla_{\boldsymbol{b}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$$

Compute gradient of hidden layer below:

$$\nabla_{\boldsymbol{h}^{(\ell-1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \boldsymbol{W}^{(\ell)\top} \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$$

Compute gradient of hidden layer below (before activation):

$$\nabla_{\boldsymbol{z}^{(\ell-1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{h}^{(\ell-1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \odot \boldsymbol{g}'(\boldsymbol{z}^{(\ell-1)}) \odot \boldsymbol{m}^{(\ell-1)}$$

end for

Outline

Initialization

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- Weights:
  - ✓ Cannot initialize to zero with tanh activation (gradients would also be all zero and we would be at saddle point)
  - ✓ Cannot initialize the weights to the same value (need to break the symmetry)
  - ✓ Random initialization (Gaussian, uniform), sampling around 0 to break symmetry
  - ✓ For ReLU activations, the mean should be a small positive number
  - ✓ Variance cannot be too high, otherwise all neuron activations will be saturated

"Glorot Initialization"

- Recipe from Glorot and Bengio (2010):

$$\boldsymbol{W}_{i,j}^{(\ell)} \sim U[-t, t], \text{ with } t = \frac{\sqrt{6}}{\sqrt{K^{(\ell)} + K^{(\ell-1)}}}$$

- Works well in practice with tanh and sigmoid activations

Training, Validation, and Test Sets

Split datasets in training, validation, and test partitions.

- Training set: serves to train the model
- Validation set: used to tune hyperparameters (learning rate, number of hidden units, regularization coefficient, dropout probability, best epoch, etc.)
- Test set: used to estimate the generalization performance

Hyperparameter Tuning: Grid Search, Random Search

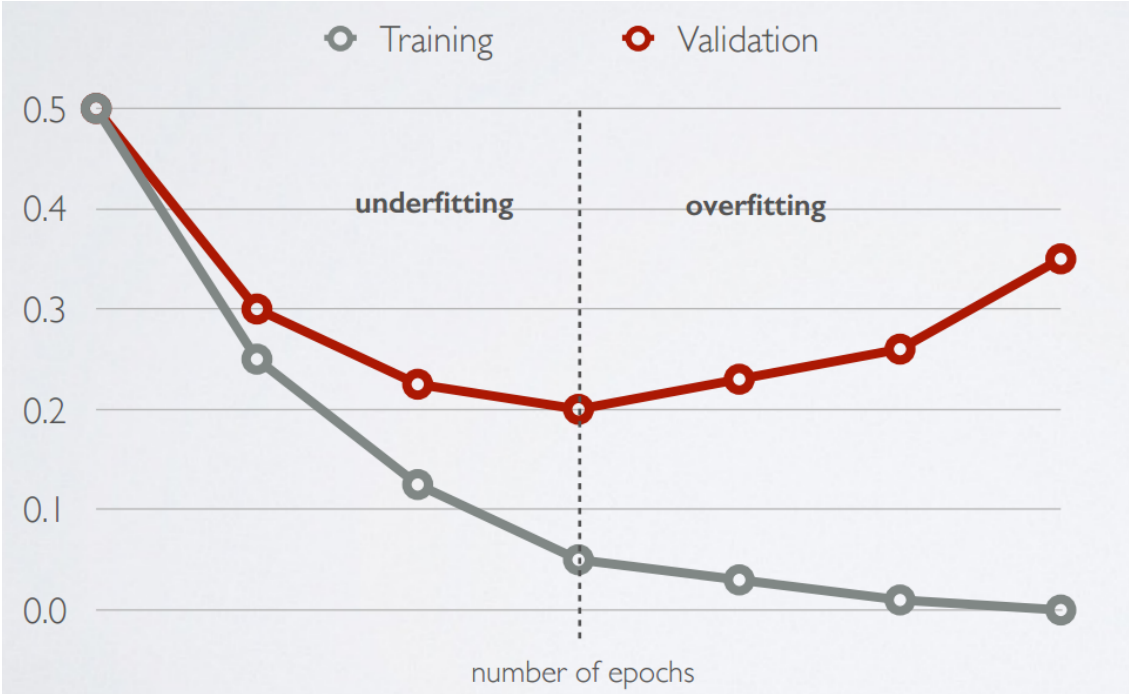
Search for the best configuration of the hyperparameters:

- Grid search: specify a set of values to test for each hyperparameter, and try all configurations of these values
- Random search: specify a distribution over the values of each hyper-parameter (e.g. uniform in some range) and sample independently each hyper-parameter to get configurations
- Bayesian optimization (Snoek et al., 2012)

We can always go back and fine-tune the grid/distributions if necessary

Early Stopping

- To select the number of epochs, stop training when validation error increases (with some look ahead)
- One common strategy (with SGD) is to halve the learning rate for every epoch where the validation error increases

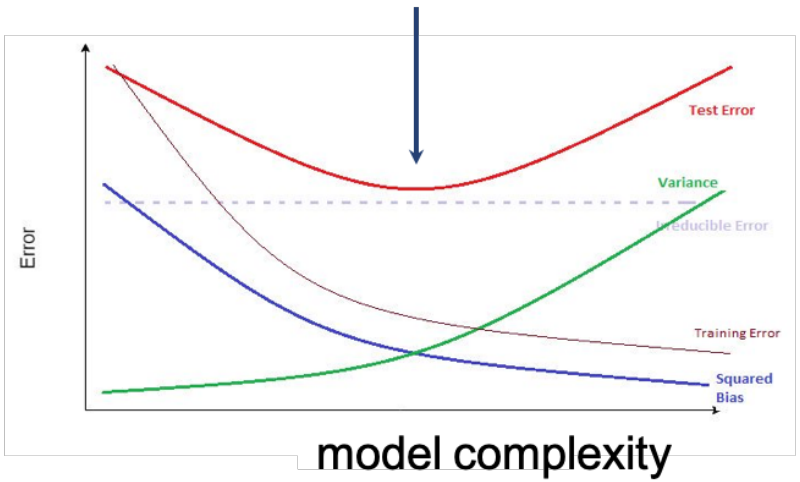


(Image credit: Hugo Larochelle)

Cross Validation

Model selection

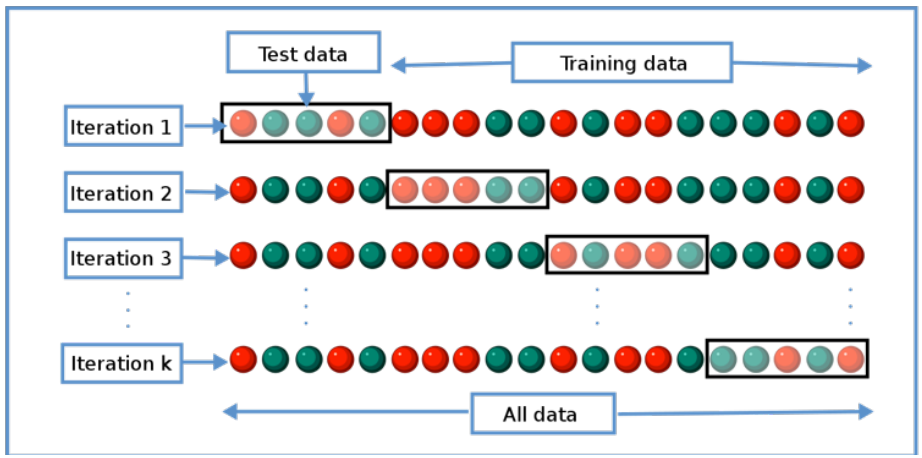
finding the sweet spot (F)



validation set:

- ✓ split data into train and validation susbsets
- ✓ train on the training subset
- ✓ test on the validation subset

cross validation (k-fold): repeat k times; average

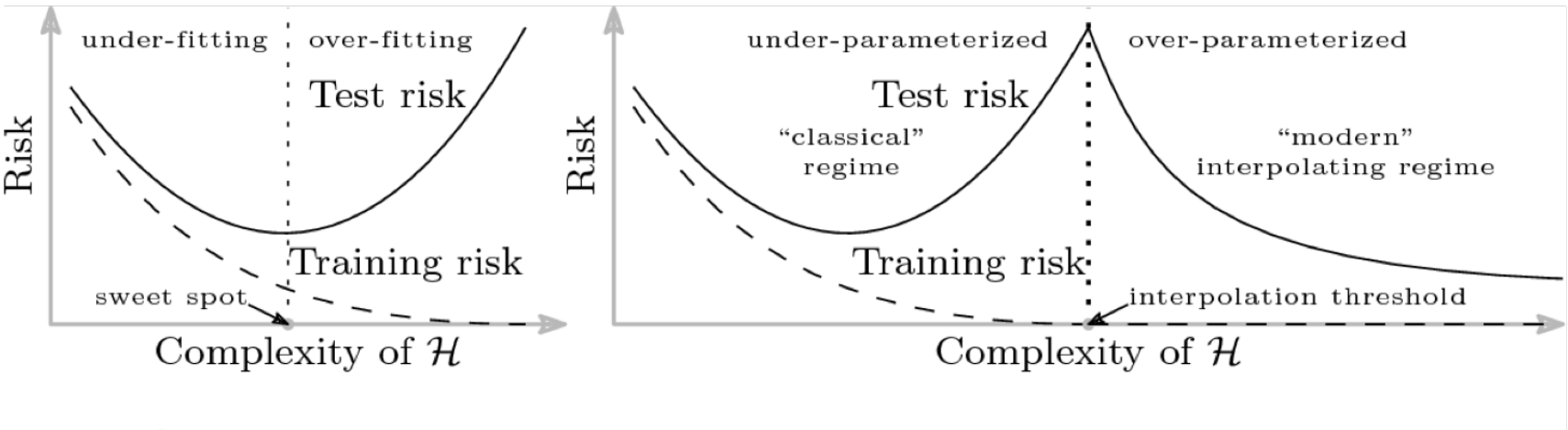


Over-parametrization

The new regime…

modern deep networks have "too many" parameters: they should overfit, …

…yet, they usually don't. Why? Ongoing research.



(illustration by Mikhail Belkin)

Tricks of the Trade

- Normalization of the data
- Decaying the learning rate
- Mini-batches
- Adaptive learning rates
- Gradient checking
- Debugging on a small dataset

Normalization of the Data

- For each input dimension: subtract the training set mean and divide by the training set standard deviation
- It makes each input dimension have zero mean, unit variance
- It can speed up training (in number of epochs)
- Doesn't work for sparse inputs (destroys sparsity)

Decaying the Learning Rate

In SGD, as we get closer to a local minimum, it makes sense to take smaller update steps (to avoid diverging)

- Start with a large learning rate (say 0.1)
- Keep it fixed while validation error keeps improving
- Divide by 2 and go back to the previous step

Mini-Batches

- Instead of updating after a single example, can aggregate a mini-batch of examples (e.g. 50–200 examples) and compute the averaged gradient for the entire mini-batch
- Less noisy than standard SGD
- Can leverage matrix-matrix computations (or tensor computations)
- Large computational speed-ups in GPUs: computation is trivially parallelizable accross the mini-batch and we can exhaust the GPU memory

Adaptive Learning Rates

Instead of using the same step size for all parameters, have one learning rate per parameter

- Adagrad (Duchi et al., 2011): learning rates are scaled by the square root of the cumulative sum of squared gradients

$$\eta^{(t)} = \eta^{(t-1)} + (\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y))^2, \qquad \bar{\nabla}_{\boldsymbol{\theta}}^{(t)} = \frac{\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y)}{\sqrt{\eta^{(t)} + \epsilon}}$$

- RMSprop (Tieleman and Hinton, 2012): instead of cumulative sum, use exponential moving average

$$\eta^{(t)} = \beta\eta^{(t-1)} + (1-\beta)(\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y))^2, \qquad \bar{\nabla}_{\boldsymbol{\theta}}^{(t)} = \frac{\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y)}{\sqrt{\eta^{(t)} + \epsilon}}$$

- Adam (Kingma and Ba, 2014): combine RMSProp with momentum

Gradient Checking

- If the training loss is not decreasing even with a very small learning rate, there's likely a bug in the gradient computation

- To debug your implementation of `fprop`/`bprop`, compute the "numeric gradient," a finite difference approximation of the true gradient:

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon}$$

Debugging on a Small Dataset

- Extract a small subset of your training set (e.g. 50 examples)
- Monitor your training loss in this set
- You should be able to overfit in this small training set
- If not, see if some units are saturated from the very first iterations (if they are, reduce the initialization variance or properly normalize your inputs)
- If the training error is bouncing up and down, decrease the learning rate

Outline

Conclusions

- Multi-layer perceptrons are universal function approximators
- However, they need to be trained
- Stochastic gradient descent is an effective training algorithm
- This is possible with the gradient backpropagation algorithm (an application of the chain rule of derivatives)
- Most current software packages represent a computation graph and implement automatic differentiation
- Dropout regularization is effective to avoid overfitting

Thank you!

Questions?

References I

Duchi, J., Hazan, E., and Singer, Y. (2011). Adaptive subgradient methods for online learning and stochastic optimization. *Journal of Machine Learning Research*, 12(Jul):2121–2159.

Glorot, X. and Bengio, Y. (2010). Understanding the difficulty of training deep feedforward neural networks. In *AISTATS*, volume 9, pages 249–256.

Hinton, G. E., Srivastava, N., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. R. (2012). Improving neural networks by preventing co-adaptation of feature detectors. *arXiv preprint arXiv:1207.0580*.

Kingma, D. and Ba, J. (2014). Adam: A Method for Stochastic Optimization. In *Proc. of International Conference on Learning Representations*.

Snoek, J., Larochelle, H., and Adams, R. P. (2012). Practical bayesian optimization of machine learning algorithms. In *Advances in neural information processing systems*, pages 2951–2959.

Srivastava, N., Hinton, G. E., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. (2014). Dropout: a simple way to prevent neural networks from overfitting. *Journal of Machine Learning Research*, 15(1):1929–1958.

Tieleman, T. and Hinton, G. (2012). Rmsprop: Divide the gradient by a running average of its recent magnitude. *COURSERA: Neural Networks for Machine Learning*, 4(2).

Wager, S., Wang, S., and Liang, P. S. (2013). Dropout training as adaptive regularization. In *Advances in neural information processing systems*, pages 351–359.

Wan, L., Zeiler, M., Zhang, S., Cun, Y. L., and Fergus, R. (2013). Regularization of neural networks using dropconnect. In *Proc. of the International Conference on Machine Learning*, pages 1058–1066.

Zeiler, M. D. and Fergus, R. (2013). Stochastic pooling for regularization of deep convolutional neural networks. *arXiv preprint arXiv:1301.3557*.