Neural Networks – Part 2

- Training Perceptrons
- Handling Multiclass Problems

CSE 4309 – Machine Learning
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Training a Neural Network

- In some cases, the training process can find the best solution using a closed-form formula.
 - Example: linear regression, for the sum-of-squares error
- In some cases, the training process can find the best weights using an iterative method.
 - Example: sequential learning for logistic regression.
- In neural networks, we **cannot** find the best weights (unless we have an astronomical amount of luck).
 - We use gradient descent to find local minima of the error function.
 - In recent years this approach has produced spectacular results in real-world applications.

Notation for Training Set

We have a set X of N training examples.

$$- X = \{x_1, x_2, ..., x_N\}$$

• Each x_n is a D-dimensional column vector.

$$- x_n = (x_{n,1}, x_{n,2}, ..., x_{n,D})'$$

- We also have a set T of N target outputs.
 - $T = \{t_1, t_2, ..., t_N\}$
 - t_n is the target output for training example x_n .
- Each t_n is a K-dimensional column vector:

$$- t_n = (t_{n,1}, t_{n,2}, ..., t_{n,K})'$$

- Note: K typically is not equal to D.
 - In your assignment, K is equal to the number of classes.
 - K is also equal to the number of units in the output layer.

- Before we discuss how to train an entire neural network, we start with a single perceptron.
- Remember: given input x_n , a perceptron computes its output z using this formula: $z(x_n) = h(b + \mathbf{w}^T x_n)$
- What are the model parameters that we want to optimize during training?

- Before we discuss how to train an entire neural network, we start with a single perceptron.
- Remember: given input x_n , a perceptron computes its output z using this formula: $z(x_n) = h(b + \mathbf{w}^T x_n)$
- What are the model parameters that we want to optimize during training?
- The weights:
 - Bias weight b.
 - Weight vector w.

Regression or Classification?

- The perceptron produces a continuous value between 0 and 1.
- Thus, perceptrons and neural networks are <u>regression</u> models, since they produce continuous outputs.
- However, perceptrons and neural networks can easily be used for classification.
- A perceptron can be treated as a <u>binary classifier</u>:
 - One class label is 0.
 - One class label is 1.
- Neural networks can do <u>multiclass classification</u> (more details on that later).

- Given input x_n , a perceptron computes its output z using this formula: $z(x_n) = h(b + \mathbf{w}^T x_n)$
- We use sum-of-squares as our error function.
- $E_n(b, w)$ is the contribution of training example x_n :

$$E_n(b, \mathbf{w}) = \frac{1}{2}(z(\mathbf{x}_n) - t_n)^2$$

- The error E over the entire training set is defined as: $E(b, \mathbf{w}) = \sum_{n=1}^{N} E_n(b, \mathbf{w})$
- Important: a single perceptron has a single output.
 - Therefore, for perceptrons (but NOT for neural networks in general), we assume that t_n is one-dimensional.

 Suppose that a perceptron is using the step function as its activation function h.

$$h(a) = \begin{cases} 0, & \text{if } a < 0 \\ 1, & \text{if } a \ge 0 \end{cases}$$

$$h(a) = \begin{cases} 0, & \text{if } a < 0 \\ 1, & \text{if } a \ge 0 \end{cases} \quad z(x) = h(b + w^T x) = \begin{cases} 0, & \text{if } b + w^T x < 0 \\ 1, & \text{if } b + w^T x \ge 0 \end{cases}$$

- Can we apply gradient descent in that case?
- No, because E(b, w) is not differentiable.
 - Small changes of b or w usually lead to no changes in $h(b + \mathbf{w}^T \mathbf{x}).$
 - The only exception is when the change in b or w causes $h(b + w^T x)$ to switch signs (from positive to negative, or from negative to positive).

• A better option is setting *h* to the sigmoid function:

$$z(\mathbf{x}) = h(b + \mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-b - \mathbf{w}^T \mathbf{x}}}$$

• Then, measured just on a single training object x_n , the error $E_n(b, \mathbf{w})$ is defined as:

$$E_n(b, \mathbf{w}) = \frac{1}{2} (t_n - z(\mathbf{x}_n))^2 = \frac{1}{2} (t_n - \frac{1}{1 + e^{-b - \mathbf{w}^T \mathbf{x}_n}})^2$$

• Reminder: if our neural network is a single perceptron, then the target output t_n **must be** one-dimensional. These formulas, so far, deal only with training a single perceptron.

Computing the Gradient

•
$$E_n(b+w) = \frac{1}{2} (t_n - z(x_n))^2 = \frac{1}{2} (t_n - \frac{1}{1+e^{-b-w^T x_n}})^2$$

- In this form, $E_n(b, w)$ is differentiable.
- If we do the calculations, the gradients turn out to be:

$$\frac{\partial E_n}{\partial b} = \frac{1}{2} \left(t_n - z(\boldsymbol{x}_n) \right) * z(\boldsymbol{x}_n) * \left(1 - z(\boldsymbol{x}_n) \right)$$

$$\frac{\partial E_n}{\partial \boldsymbol{w}} = \frac{1}{2} \left(t_n - z(\boldsymbol{x}_n) \right) * z(\boldsymbol{x}_n) * \left(1 - z(\boldsymbol{x}_n) \right) * \boldsymbol{x}_n$$

Computing the Gradient

•
$$E_n(b+w) = \frac{1}{2} (t_n - z(x_n))^2 = \frac{1}{2} (t_n - \frac{1}{1+e^{-b-w^T x_n}})^2$$

• From the previous slide, the gradients are:

$$\frac{\partial E_n}{\partial b} = \frac{1}{2} \left(t_n - z(\mathbf{x}_n) \right) * z(\mathbf{x}_n) * \left(1 - z(\mathbf{x}_n) \right)$$

$$\frac{\partial E_n}{\partial \mathbf{w}} = \frac{1}{2} \left(t_n - z(\mathbf{x}_n) \right) * z(\mathbf{x}_n) * \left(1 - z(\mathbf{x}_n) \right) * \mathbf{x}_n$$

• Note that $\frac{\partial E_n}{\partial w}$ is a D-dimensional vector. It is a scalar (shown in red) multiplied by vector x_n .

Weight Update

$$\frac{\partial E_n}{\partial h} = \frac{1}{2} (t_n - z(\mathbf{x}_n)) * z(\mathbf{x}_n) * (1 - z(\mathbf{x}_n))$$

$$\frac{\partial E_n}{\partial \mathbf{w}} = \frac{1}{2} \left(t_n - z(\mathbf{x}_n) \right) * z(\mathbf{x}_n) * \left(1 - z(\mathbf{x}_n) \right) * \mathbf{x}_n$$

 So, we update the bias weight b and weight vector w as follows:

$$b = b - \eta * (t_n - z(\mathbf{x}_n)) * z(\mathbf{x}_n) * (1 - z(\mathbf{x}_n))$$

$$\mathbf{w} = \mathbf{w} - \eta * (t_n - z(\mathbf{x}_n)) * z(\mathbf{x}_n) * (1 - z(\mathbf{x}_n)) * \mathbf{x}_n$$

Weight Update

• (From previous slide) Update formulas:

$$b = b - \eta * (t_n - z(x_n)) * z(x_n) * (1 - z(x_n))$$

$$w = w - \eta * (t_n - z(x_n)) * z(x_n) * (1 - z(x_n)) * x_n$$

- As before, η is the learning rate parameter.
 - It is a positive real number that should be chosen carefully, so as not to be too big or too small.
- In terms of individual weights w_d , the update rule is:

$$w_d = w_d - \eta * (t_n - z(\mathbf{x}_n)) * z(\mathbf{x}_n) * (1 - z(\mathbf{x}_n)) * x_{n,d}$$

Perceptron Learning - Summary

- Input: Training inputs x_1, \dots, x_N , target outputs t_1, \dots, t_N
 - For a binary classification problem, each t_n is set to 0 or 1.
- 1. Initialize b and each w_d to small random numbers.
 - For example, set b and each w_d to a random value between -0.1 and 0.1
- 2. For n = 1 to N:
 - a) Compute $z(x_n)$.
 - b) $b = b \eta * (t_n z(x_n)) * z(x_n) * (1 z(x_n))$
 - c) For d = 0 to D: $w_d = w_d - \eta * (t_n - z(x_n)) * z(x_n) * (1 - z(x_n)) * x_{n,d}$
- 3. If some stopping criterion has been met, exit.
- 4. Else, go to step 2.

Stopping Criterion

- At step 3 of the perceptron learning algorithm, we need to decide whether to stop or not.
- One thing we can do is:
 - Compute the cumulative squared error E(w) of the perceptron at that point:

$$E(b, \mathbf{w}) = \sum_{n=1}^{N} E_n(b, \mathbf{w}) = \sum_{n=1}^{N} \left\{ \frac{1}{2} (t_n - z(\mathbf{x}_n))^2 \right\}$$

- Compare the current value of $E(b, \mathbf{w})$ with the value of $E(b, \mathbf{w})$ computed at the previous iteration.
- If the difference is too small (e.g., smaller than 0.00001) we stop.

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Using Perceptrons for Multiclass Problems

- "Multiclass" means that we have more than two classes.
- A perceptron outputs a number between 0 and 1.
- This is sufficient only for binary classification problems.
- For more than two classes, there are many different options.
- We will follow a general approach called <u>one-versus-all</u> <u>classification</u> (also known as OVA classification).
 - This approach is a general method, that can be combined with various binary classification methods, so as to solve multiclass problems. Here we see the method applied to perceptrons.

A Multiclass Example

Suppose we have this training set:

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, q_1 = dog$$

$$-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, q_2 = dog$$

$$-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, q_3 = cat$$

$$-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, q_4 = fox$$

$$-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, q_5 = cat$$

$$-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, q_6 = fox$$

- In this training set:
 - We have three classes.
 - Each training input x_n is a five-dimensional vector.
 - The class labels q_n are strings.

Suppose we have this training set:

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, \quad q_1 = \text{dog}, \quad s_1 = 1$$

$$-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, \quad q_2 = \text{dog}, \quad s_2 = 1$$

$$-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, \quad q_3 = \text{cat}, \quad s_3 = 2$$

$$-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, \quad q_4 = \text{fox}, \quad s_4 = 3$$

$$-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, \quad q_5 = \text{cat}, \quad s_5 = 2$$

$$-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, \quad q_6 = \text{fox}, \quad s_6 = 3$$

• Step 1:

— Generate new class labels s_n , where classes are numbered sequentially starting from 1. Thus, in our example, the class labels become 1, 2, 3.

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, s_1 = 1$$

$$-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, s_2 = 1$$

$$-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, s_3 = 2$$

$$-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, s_4 = 3$$

$$-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, s_5 = 2$$

$$-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, s_6 = 3$$

- Step 2: Convert each label s_n to a **one-hot vector** t_n .
 - Vector t_n has as many dimensions as the number of classes.
 - How many dimensions should we use in our example?

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, s_1 = 1
-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, s_2 = 1
-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, s_3 = 2
-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, s_4 = 3
-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, s_5 = 2
-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, s_6 = 3
$$t_1 = (?,?,?)^T$$

$$t_2 = (?,?,?)^T$$

$$t_3 = (?,?,?)^T$$

$$t_4 = (?,?,?)^T$$

$$t_5 = (?,?,?)^T$$$$

- Step 2: Convert each label s_n to a **one-hot vector** t_n .
 - Vector t_n has as many dimensions as the number of classes.
 - ullet In our example we have three classes, so each $oldsymbol{t}_n$ is 3-dimensional.
 - If $s_n = i$, then set the i-th dimension of t_n to 1.
 - Otherwise, set the i-th dimension of t_n to 0.

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, \quad s_1 = 1$$

$$-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, \quad s_2 = 1$$

$$-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, \quad s_3 = 2$$

$$-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, \quad s_4 = 3$$

$$-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, \quad s_5 = 2$$

$$-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, \quad s_6 = 3$$

$$t_1 = (1, 0, 0)^T$$

$$t_2 = (1, 0, 0)^T$$

$$t_3 = (0, 1, 0)^T$$

$$t_4 = (0, 0, 1)^T$$

$$t_5 = (0, 1, 0)^T$$

- Step 2: Convert each label s_n to a **one-hot vector** t_n .
 - Vector t_n has as many dimensions as the number of classes.
 - ullet In our example we have three classes, so each $oldsymbol{t}_n$ is 3-dimensional.
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 - Otherwise, set the i-th dimension of t_n to 0.

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, \quad s_1 = 1$$

$$-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, \quad s_2 = 1$$

$$-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, \quad s_3 = 2$$

$$-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, \quad s_4 = 3$$

$$-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, \quad s_5 = 2$$

$$-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, \quad s_6 = 3$$

$$t_1 = (1, 0, 0)^T$$

$$t_2 = (1, 0, 0)^T$$

$$t_3 = (0, 1, 0)^T$$

$$t_4 = (0, 0, 1)^T$$

$$t_5 = (0, 1, 0)^T$$

- Step 3: Train three separate perceptrons (as many as the number of classes).
- For training the <u>first</u> perceptron, use the <u>first</u> dimension of each t_n as target output for x_n .

Training Set for the First Perceptron

Training set used to train the first perceptron:

$$- x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, t_1 = 1$$

$$- x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, t_2 = 1$$

$$- x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, t_3 = 0$$

$$- x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, t_4 = 0$$

$$- x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, t_5 = 0$$

$$- x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, t_6 = 0$$

- Essentially, the first perceptron is trained to output "1" when:
 - The original class label q_n is "dog".
 - The sequentially numbered class label s_n is 1.

Training set for the multiclass problem:

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, \quad s_1 = 1 \qquad t_1 = (1, 0, 0)^T
-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, \quad s_2 = 1 \qquad t_2 = (1, 0, 0)^T
-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, \quad s_3 = 2 \qquad t_3 = (0, 1, 0)^T
-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, \quad s_4 = 3 \qquad t_4 = (0, 0, 1)^T
-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, \quad s_5 = 2 \qquad t_5 = (0, 1, 0)^T
-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, \quad s_6 = 3 \qquad t_6 = (0, 0, 1)^T$$

- Step 3: Train three separate perceptrons (as many as the number of classes).
- For training the <u>second</u> perceptron, use the <u>second</u> dimension of each t_n as target output for x_n .

Training Set for the Second Perceptron

Training set used to train the second perceptron:

$$- x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, t_1 = 0$$

$$- x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, t_2 = 0$$

$$- x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, t_3 = 1$$

$$- x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, t_4 = 0$$

$$- x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, t_5 = 1$$

$$- x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, t_6 = 0$$

- Essentially, the second perceptron is trained to output "1" when:
 - The original class label q_n is "cat".
 - The sequentially numbered class label s_n is 2.

Training set for the multiclass problem:

$$-x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, s_1 = 1 t_1 = (1, 0, 0)^T
-x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, s_2 = 1 t_2 = (1, 0, 0)^T
-x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, s_3 = 2 t_3 = (0, 1, 0)^T
-x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, s_4 = 3 t_4 = (0, 0, 1)^T
-x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, s_5 = 2 t_5 = (0, 1, 0)^T
-x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, s_6 = 3 t_6 = (0, 0, 1)^T$$

- Step 3: Train three separate perceptrons (as many as the number of classes).
- For training the <u>third</u> perceptron, use the <u>third</u> dimension of each t_n as target output for x_n .

Training Set for the Third Perceptron

Training set used to train the third perceptron:

$$- x_1 = (0.5, 2.4, 8.3, 1.2, 4.5)^T, t_1 = 0$$

$$- x_2 = (3.4, 0.6, 4.4, 6.2, 1.0)^T, t_2 = 0$$

$$- x_3 = (4.7, 1.9, 6.7, 1.2, 3.9)^T, t_3 = 0$$

$$- x_4 = (2.6, 1.3, 9.4, 0.7, 5.1)^T, t_4 = 1$$

$$- x_5 = (8.5, 4.6, 3.6, 2.0, 6.2)^T, t_5 = 0$$

$$- x_6 = (5.2, 8.1, 7.3, 4.2, 1.6)^T, t_6 = 1$$

- Essentially, the third perceptron is trained to output "1" when:
 - The original class label q_n is "fox".
 - The sequentially numbered class label s_n is 3.

One-Versus-All Perceptrons: Recap

- Suppose we have K classes $C_1, ..., C_K$, where K > 2.
- We have training inputs x_1, \dots, x_N , and target values t_1, \dots, t_N .
- Each target value t_n is a K-dimensional vector:
 - $\mathbf{t}_n = (t_{n,1}, t_{n,2}, ..., t_{n,K})$
 - $-t_{n,k} = 0$ if the class of x_n is not C_k .
 - $-t_{n,k}=1$ if the class of x_n is C_k .
- For each class C_k , train a perceptron z_k by using $t_{n,k}$ as the target value for \boldsymbol{x}_n .
 - So, perceptron z_k is trained to recognize if an object belongs to class C_k or not.
 - In total, we train K perceptrons, one for each class.

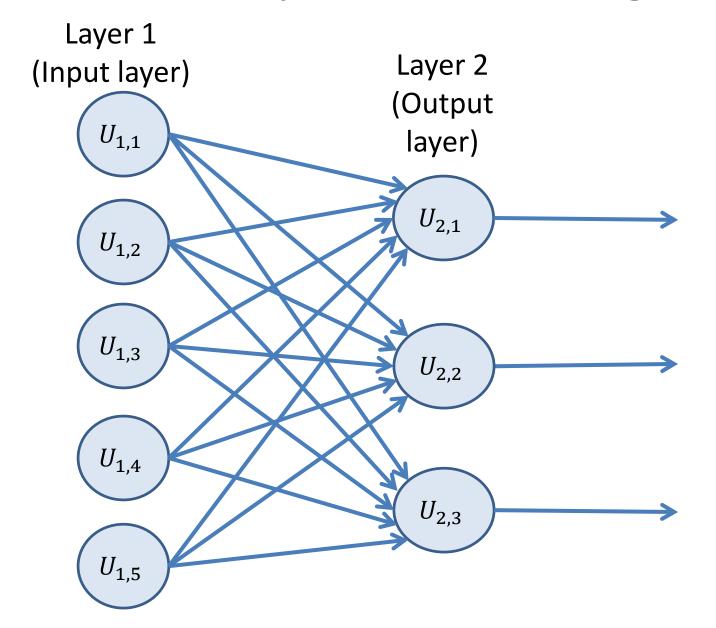
One-Versus-All Perceptrons

- To classify a test pattern x:
 - Compute the responses $z_k(x)$ for all K perceptrons.
 - Find the perceptron z_{k*} such that the value $z_{k*}(x)$ is higher than all other responses.
 - Output that the class of x is C_{k*} .
- In summary: we assign x to the class whose perceptron produced the highest output value for x.

Multiclass Neural Networks

- For perceptrons, we saw that we can perform multiclass (i.e., for more than two classes) classification using the one-versus-all (OVA) approach:
 - We train one perceptron for each class.
- These multiple perceptrons can also be thought of as a <u>single neural network</u>.

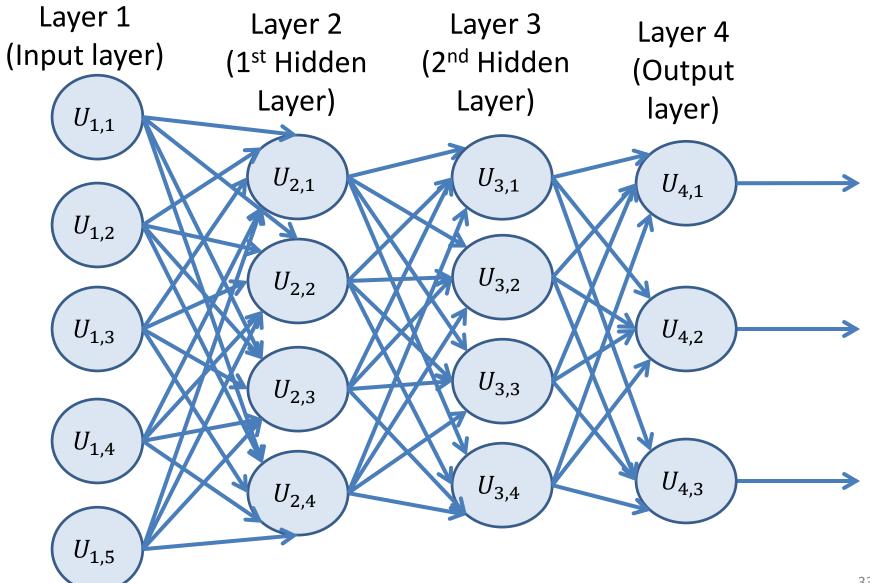
OVA Perceptrons as a Single Network



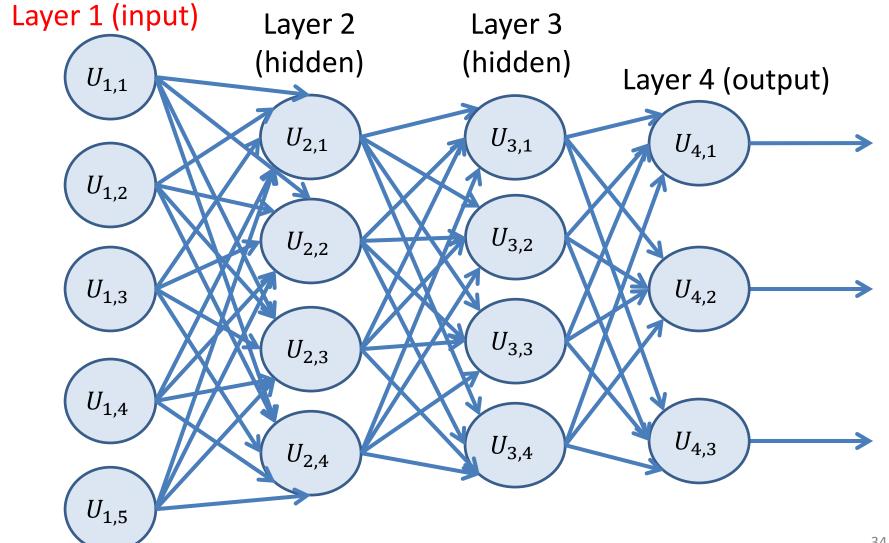
Multiclass Neural Networks

- For perceptrons, we saw that we can perform multiclass (i.e., for more than two classes) classification using the one-versus-all (OVA) approach:
 - We train one perceptron for each class.
- These multiple perceptrons can also be thought of as a <u>single neural network</u>.
- In the simplest case, a neural network designed to recognize multiple classes looks like the previous example.
- In the general case, there are also hidden layers.

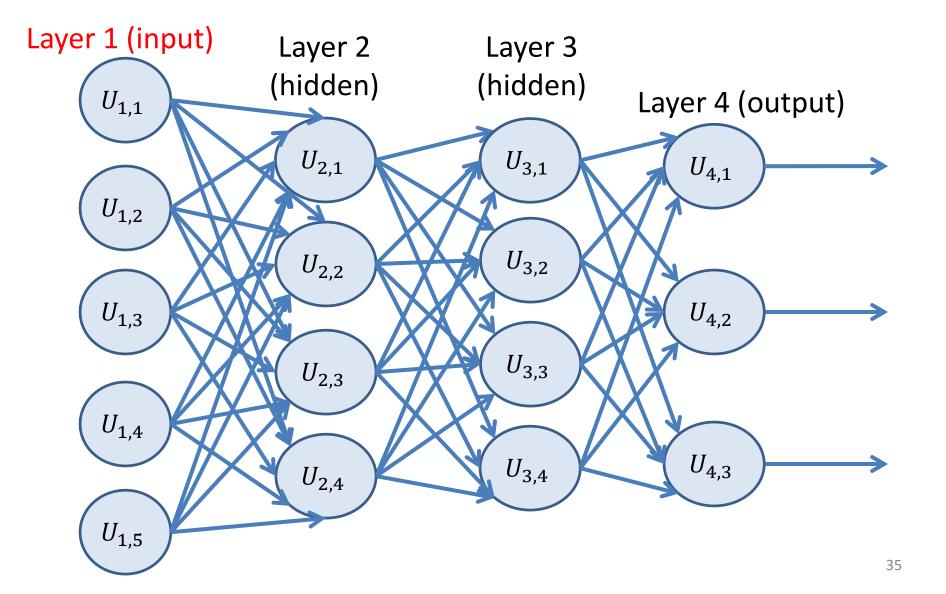
A Network for Our Example



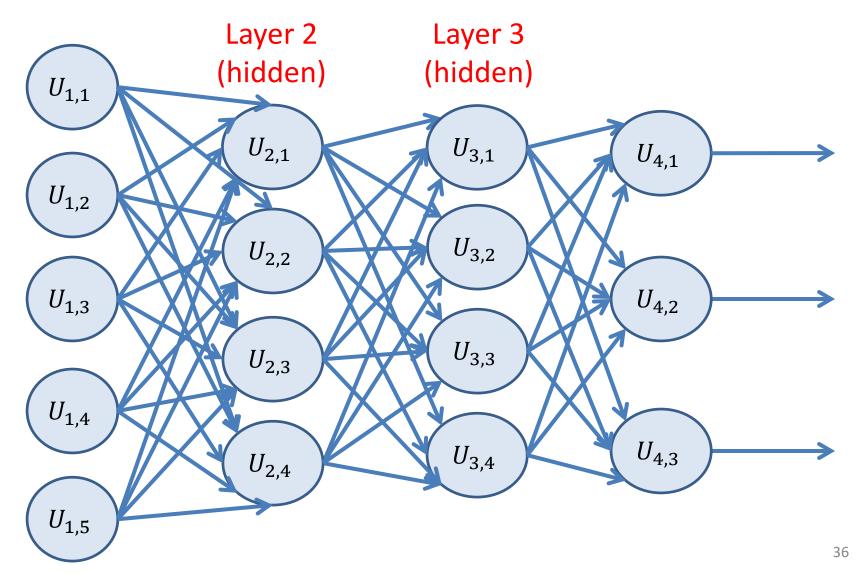
Input Layer: How many units does it have? Could we have a different number? Is the number of input units a hyperparameter?



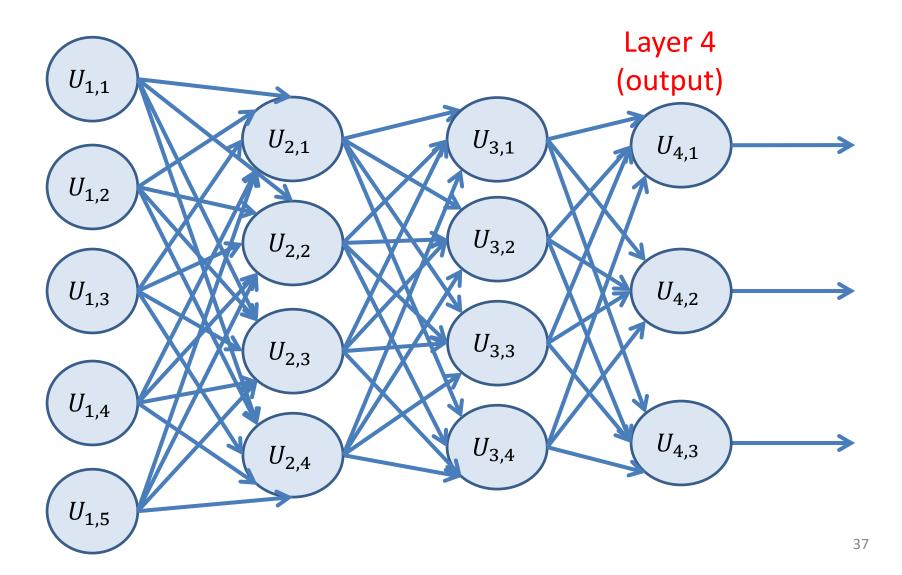
In our example, the input layer it <u>must</u> have five units, because each input is five-dimensional. We don't have a choice.



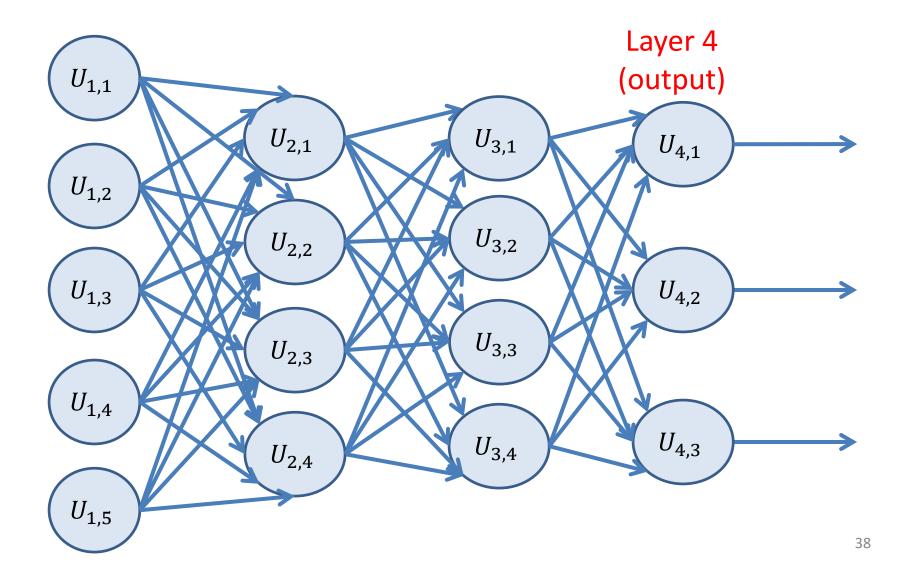
- This network has two hidden layers, with four units per layer.
- The number of hidden layers and the number of units per layer are hyperparameters, they can take different values.



Output Layer: How many units does it have? Could we have a different number? Is the number of output units a hyperparameter?

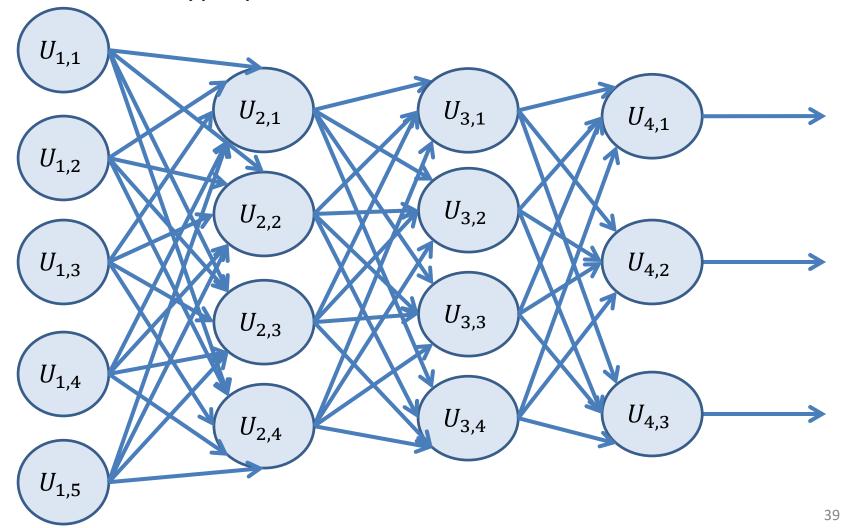


 In our example, the output layer <u>must</u> have three units, because we want to recognize three different classes (dog, cat, fox). We have no choice.



Network connectivity:

- In this neural network, at layers 2, 3, 4, every unit receives as input the output of ALL units in the previous layer.
- This is also a hyperparameter, it doesn't have to be like that.



Next: Training

- The next set of slides will describe how to train such a network.
- Training a neural network is done using gradient descent.
- The specific method is called **backpropagation**, but it really is just a straightforward application of gradient descent for neural networks.