Advanced Machine Learning
Lecture 12

Neural Networks

10.12.2015

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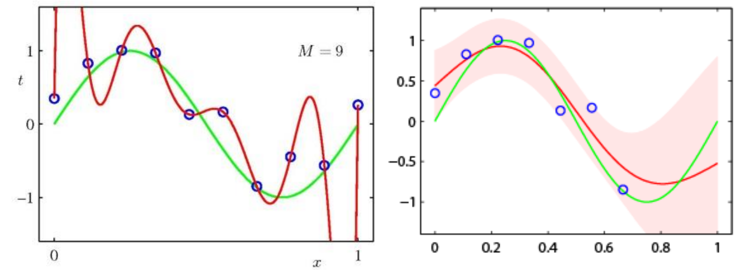
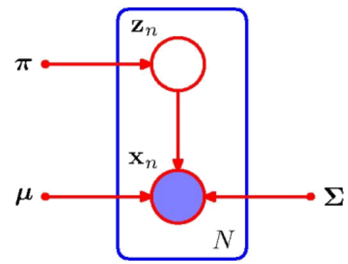
This Lecture: *Advanced Machine Learning*

- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Gaussian Processes

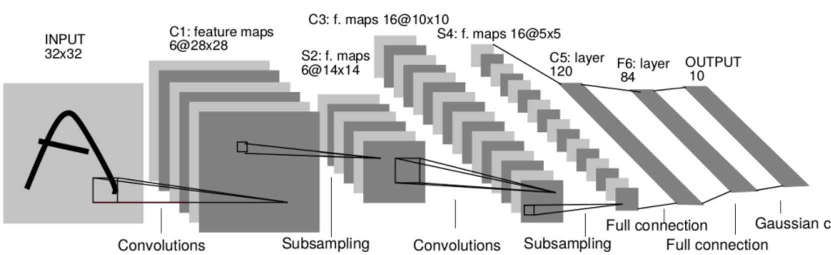
$$f : \mathcal{X} \rightarrow \mathbb{R}$$



- Learning with Latent Variables
  - Prob. Distributions & Approx. Inference
  - Mixture Models
  - EM and Generalizations



- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation
  - CNNs, RNNs, RBMs, etc.



Recap: Generalized Linear Discriminants

- Extension with non-linear basis functions
  - Transform vector $\mathbf{x}$ with M nonlinear basis functions $\phi_j(\mathbf{x})$:

$$y_k(\mathbf{x}) = g\left(\sum_{j=1}^{M} w_{kj}\phi_j(\mathbf{x}) + w_{k0}\right)$$

  - Basis functions $\phi_j(\mathbf{x})$ allow non-linear decision boundaries.
  - Activation function $g(\,\cdot\,)$ bounds the influence of outliers.
  - Disadvantage: minimization no longer in closed form.

- Notation

$$y_k(\mathbf{x}) = g\left(\sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})\right)$$

with $\phi_0(\mathbf{x}) = 1$

Recap: Gradient Descent

- Iterative minimization
  - Start with an initial guess for the parameter values $w_{kj}^{(0)}$.
  - Move towards a (local) minimum by following the gradient.
- Basic strategies
  - "Batch learning"
    $$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$
  - "Sequential updating"
    $$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

where $$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

Recap: Gradient Descent

- **Example: Quadratic error function**

$$E(\mathbf{w}) = \sum_{n=1}^{N} \left(y(\mathbf{x}_n; \mathbf{w}) - \mathbf{t}_n\right)^2$$

- **Sequential updating leads to delta rule (=LMS rule)**

$$\begin{aligned} w_{kj}^{(\tau+1)} &= w_{kj}^{(\tau)} - \eta\left(y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn}\right)\phi_j(\mathbf{x}_n) \\ &= w_{kj}^{(\tau)} - \eta\delta_{kn}\phi_j(\mathbf{x}_n) \end{aligned}$$

  - **where**

$$\delta_{kn} = y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn}$$

$\Rightarrow$ **Simply feed back the input data point, weighted by the classification error.**

Recap: Probabilistic Discriminative Models

- Consider models of the form

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma(\mathrm{w}^T\phi)$$

with

$$p(\mathcal{C}_2|\phi) = 1 - p(\mathcal{C}_1|\phi)$$

- This model is called logistic regression.

- Properties
  - Probabilistic interpretation
  - But discriminative method: only focus on decision hyperplane
  - Advantageous for high-dimensional spaces, requires less parameters than explicitly modeling $p(\phi|\mathcal{C}_k)$ and $p(\mathcal{C}_k)$.

Recap: Logistic Regression

- **Let's consider a data set $\{\phi_n, t_n\}$ with $n = 1,\ldots,N$, where $\phi_n = \phi(\mathbf{x}_n)$ and $t_n \in \{0,1\}$, $\mathbf{t} = (t_1,\ldots,t_N)^T$.**
- **With $y_n = p(\mathcal{C}_1|\phi_n)$, we can write the likelihood as**

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} \{1 - y_n\}^{1-t_n}$$

- **Define the error function as the negative log-likelihood**

$$\begin{aligned} E(\mathbf{w}) &= -\ln p(\mathbf{t}|\mathbf{w}) \\ &= -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\} \end{aligned}$$

  - **This is the so-called cross-entropy error function.**

Recap: Gradient of the Error Function

- **Gradient for logistic regression**

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n)\phi_n$$

- **This is the same result as for the Delta (=LMS) rule**

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta(y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn})\phi_j(\mathbf{x}_n)$$

- **We can use this to derive a sequential estimation algorithm.**
  - However, this will be quite slow…
  - More efficient to use 2nd-order Newton-Raphson ⇒ IRLS

Recap: Softmax Regression

- **Multi-class generalization of logistic regression**
  - **In logistic regression, we assumed binary labels $t_n \in \{0, 1\}$**
  - **Softmax generalizes this to K values in 1-of-K notation.**

$$\mathbf{y}(\mathbf{x};\mathbf{w}) = \begin{bmatrix} P(y=1|\mathbf{x};\mathbf{w}) \\ P(y=2|\mathbf{x};\mathbf{w}) \\ \vdots \\ P(y=K|\mathbf{x};\mathbf{w}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{K}\exp(\mathbf{w}_j^\top \mathbf{x})} \begin{bmatrix} \exp(\mathbf{w}_1^\top \mathbf{x}) \\ \exp(\mathbf{w}_2^\top \mathbf{x}) \\ \vdots \\ \exp(\mathbf{w}_K^\top \mathbf{x}) \end{bmatrix}$$

  - **This uses the softmax function**

$$\frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

  - **Note: the resulting distribution is normalized.**

Recap: Softmax Regression Cost Function

- **Logistic regression**
  - Alternative way of writing the cost function

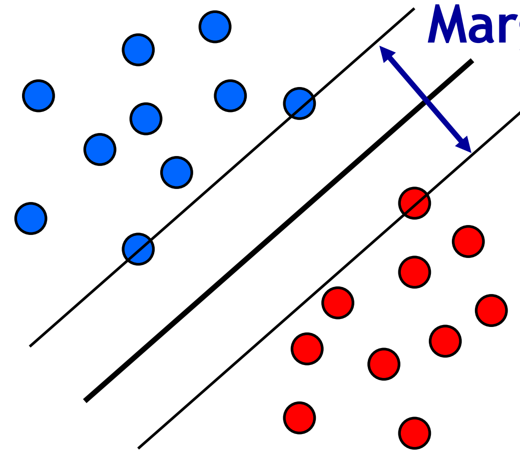
$$E(\mathbf{w}) = -\sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$
$$= -\sum_{n=1}^{N}\sum_{k=0}^{1}\{\mathbb{I}(t_n = k)\ln P(y_n = k|\mathbf{x}_n;\mathbf{w})\}$$

- **Softmax regression**
  - Generalization to K classes using indicator functions.

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K}\left\{\mathbb{I}(t_n = k)\ln\frac{\exp(\mathbf{w}_k^\top\mathbf{x})}{\sum_{j=1}^{K}\exp(\mathbf{w}_j^\top\mathbf{x})}\right\}$$

$$\nabla_{\mathbf{w}_k}E(\mathbf{w}) = -\sum_{n=1}^{N}\left[\mathbb{I}(t_n = k)\ln P(y_n = k|\mathbf{x}_n;\mathbf{w})\right]$$

Side Note: Support Vector Machine (SVM)



- Basic idea
  - The SVM tries to find a classifier which maximizes the margin between pos. and neg. data points.
  - Up to now: consider linear classifiers

$$\mathbf{w}^{\mathrm{T}}\mathbf{x} + b = 0$$

- Formulation as a convex optimization problem
  - Find the hyperplane satisfying

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

under the constraints

$$t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

based on training data points $\mathbf{x}_n$ and target values $t_n \in \{-1, 1\}$.

SVM – Analysis

- **Traditional soft-margin formulation**

$$\min_{\mathbf{w}\in\mathbb{R}^D,\, \xi_n\in\mathbb{R}^+} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

"Maximize the margin"

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1-\xi_n$$

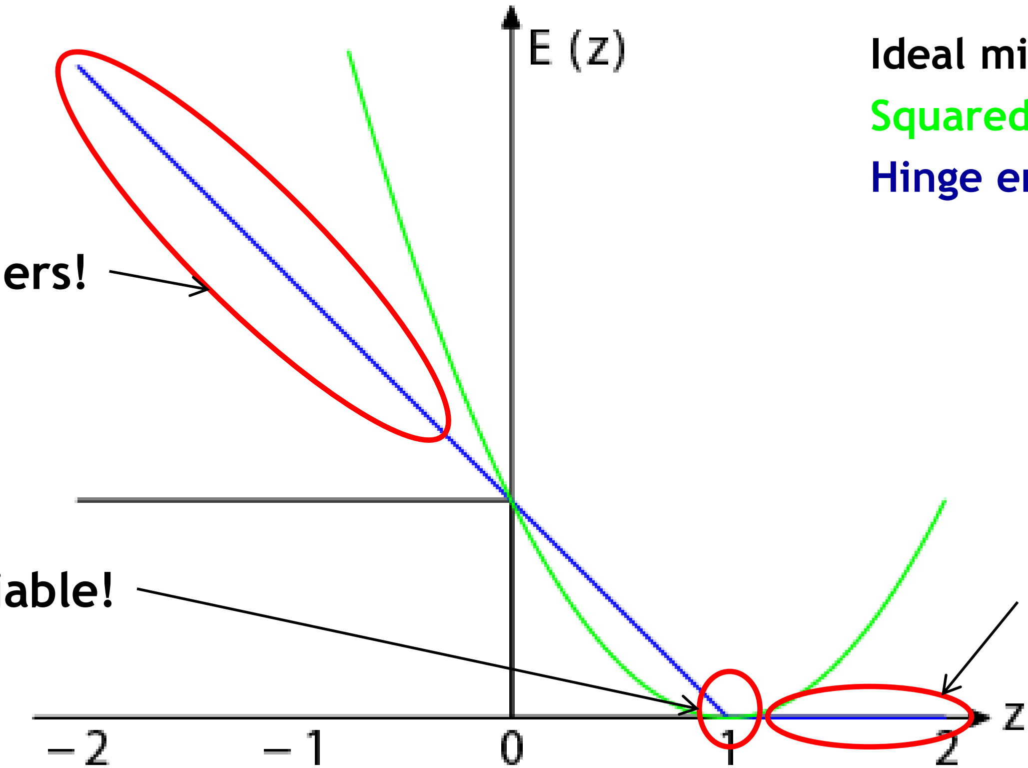
"Most points should be on the correct side of the margin"

- **Different way of looking at it**
  - We can reformulate the constraints into the objective function.

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L}_2 \text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1-t_n y(\mathbf{x}_n)]_+}_{\text{"Hinge loss"}}$$

where $[x]_+ := \max\{0,x\}$.

SVM Error Function (Loss Function)



- "Hinge error" used in SVMs
  - Zero error for points outside the margin ($z_n > 1$).
  - Linearly increasing error for misclassified points ($z_n < 1$).

  $\Rightarrow$ Leads to sparse solutions, not sensitive to outliers.
  - Not differentiable around $z_n = 1$ $\Rightarrow$ Cannot be optimized directly.

Image source: Bishop, 2006

SVM – Discussion

- SVM optimization function

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L}_2 \text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{Hinge loss}}$$

- Hinge loss enforces sparsity
  - Only a subset of training data points actually influences the decision boundary.
  - This is different from sparsity obtained through the regularizer! There, only a subset of input dimensions are used.
  - Unconstrained optimization, but non-differentiable function.
  - Solve, e.g. by *subgradient descent*
  - Currently most efficient: *stochastic gradient descent*

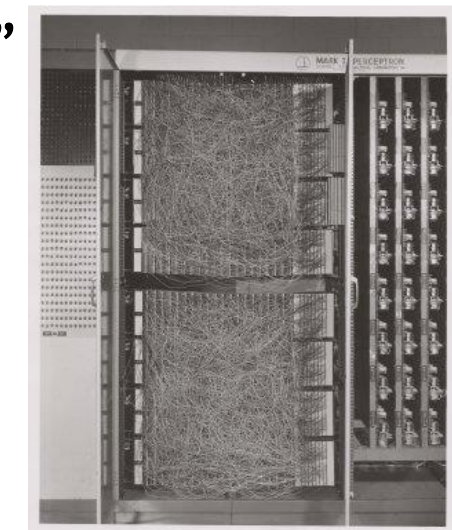
Topics of This Lecture

- A Short History of Neural Networks
- Perceptrons
  - Definition
  - Loss functions
  - Regularization
  - Limits
- Multi-Layer Perceptrons
  - Definition
  - Learning

A Brief History of Neural Networks

1957 Rosenblatt invents the Perceptron

- And a cool learning algorithm: "Perceptron Learning"
- Hardware implementation "Mark I Perceptron" for 20×20 pixel image analysis



The New York Times

"The embryo of an electronic computer that [...] will be able to walk, talk, see, write, reproduce itself and be conscious of its existence."

Image source: Wikipedia, clipartpanda.com

A Brief History of Neural Networks

1957 Rosenblatt invents the Perceptron

1969 Minsky & Papert

- They showed that (single-layer) Perceptrons cannot solve all problems.
- This was misunderstood by many that they were worthless.

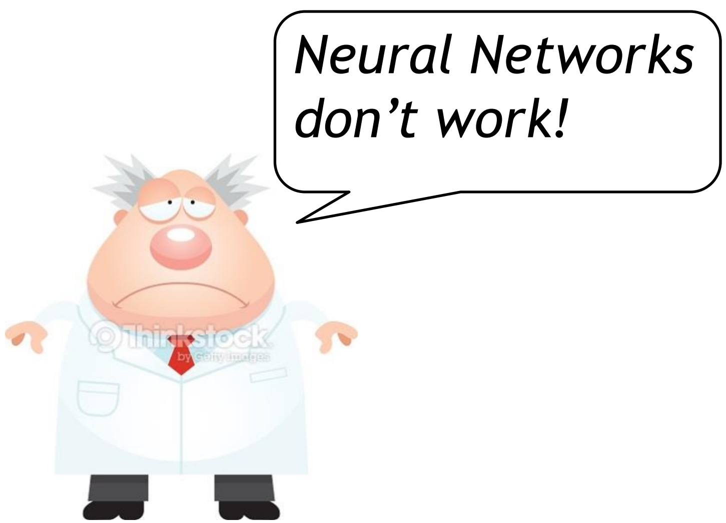


Image source: colourbox.de, thinkstock

A Brief History of Neural Networks

1957 Rosenblatt invents the Perceptron

1969 Minsky & Papert

1980s Resurgence of Neural Networks

- Some notable successes with multi-layer perceptrons.
- Backpropagation learning algorithm

OMG! They work like the human brain!

Oh no! Killer robots will achieve world domination!

Image sources: clipartpanda.com, cliparts.co

A Brief History of Neural Networks

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1980s Resurgence of Neural Networks

- Some notable successes with multi-layer perceptrons.
- Backpropagation learning algorithm
- But they are hard to train, tend to overfit, and have unintuitive parameters.
- So, the excitement fades again.

Image source: clipartof.com, colourbox.de

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1995+ Interest shifts to other learning methods

- Notably Support Vector Machines
- Machine Learning becomes a discipline of its own.

Image source: clipartof.com

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- Notably Support Vector Machines
- Machine Learning becomes a discipline of its own.
- The general public and the press still love Neural Networks.

I'm doing Machine Learning.

So, you're using Neural Networks?

Actually…

A Brief History of Neural Networks

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1980s Resurgence of Neural Networks

1995+ Interest shifts to other learning methods

2005+ Gradual progress

- Better understanding how to successfully train deep networks
- Availability of large datasets and powerful GPUs
- Still largely under the radar for many disciplines applying ML

Are you using Neural Networks?

Come on. Get real!

A Brief History of Neural Networks

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2012 Breakthrough results

- ImageNet Large Scale Visual Recognition Challenge
- A ConvNet halves the error rate of dedicated vision approaches.
- Deep Learning is widely adopted.

Image source: clipartpanda.com, clipartof.com

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- A Short History of Neural Networks
- Perceptrons
  - Definition
  - Loss functions
  - Regularization
  - Limits
- Multi-Layer Perceptrons
  - Definition
  - Learning

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Perceptrons (Rosenblatt 1957)

- Standard Perceptron

- Input Layer
  - Hand-designed features based on common sense
- Outputs
  - Linear outputs

$$y(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$$

  Logistic outputs

$$y(\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x} + w_0)$$

- Learning = Determining the weights $\mathbf{w}$

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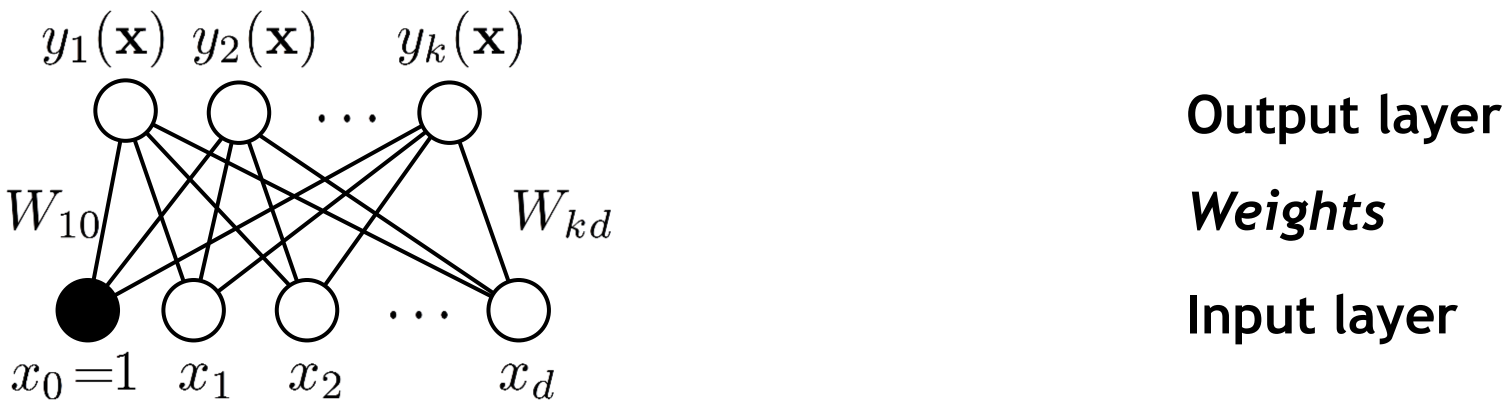
Extension: Multi-Class Networks

- One output node per class



- Outputs
  - Linear outputs

$$y_k(\mathbf{x}) = \sum_{i=0}^{d} W_{ki} x_i$$

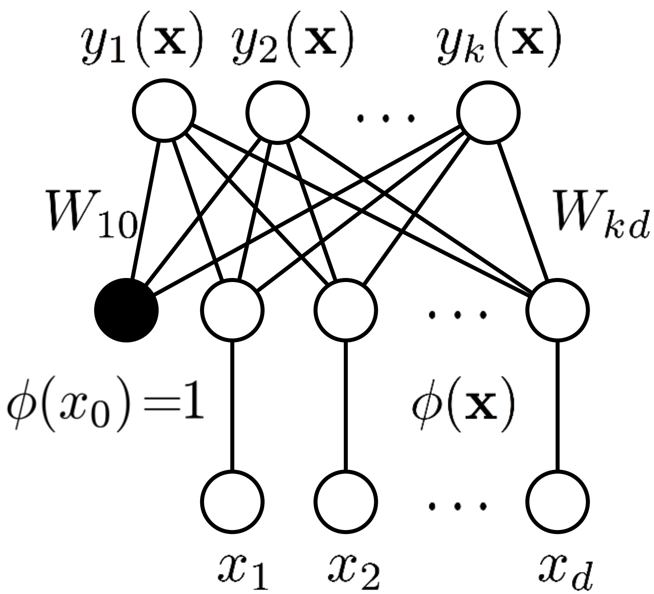
Logistic outputs

$$y_k(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} W_{ki} x_i\right)$$

⇒ Can be used to do **multidimensional linear regression** or **multiclass classification**.

Extension: Non-Linear Basis Functions

- **Straightforward generalization**



Output layer

Weights

Feature layer

Mapping (fixed)

Input layer

- **Outputs**
  - Linear outputs

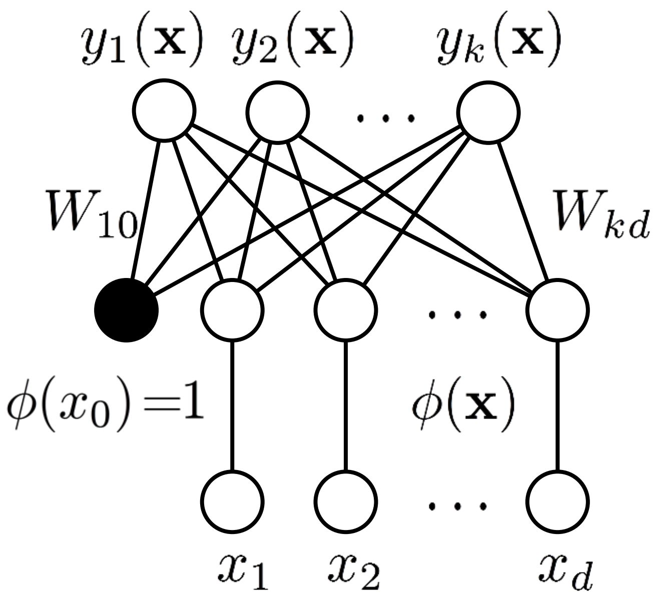
$$y_k(\mathbf{x}) = \sum_{i=0}^{d} W_{ki}\phi(x_i)$$

Logistic outputs

$$y_k(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} W_{ki}\phi(x_i)\right)$$

Extension: Non-Linear Basis Functions

- Straightforward generalization



Output layer

Weights

Feature layer

Mapping (fixed)

Input layer

- Remarks
  - Perceptrons are generalized linear discriminants!
  - Everything we know about the latter can also be applied here.
  - Note: feature functions $\phi(\mathbf{x})$ are kept fixed, not learned!

Perceptron Learning

- Very simple algorithm
- Process the training cases in some permutation
  - If the output unit is correct, leave the weights alone.
  - If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
  - If the output unit incorrectly outputs a one, subtract the input vector from the weight vector.
- This is guaranteed to converge to a correct solution if such a solution exists.

Perceptron Learning

- Let's analyze this algorithm...
- Process the training cases in some permutation
  - If the output unit is correct, leave the weights alone.
  - If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
  - If the output unit incorrectly outputs a one, subtract the input vector from the weight vector.
- Translation

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)}$$

Perceptron Learning

- Let's analyze this algorithm...
- Process the training cases in some permutation
  - If the output unit is correct, leave the weights alone.
  - If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
  - If the output unit incorrectly outputs a one, subtract the input vector from the weight vector.
- Translation

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left(y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn} \right) \phi_j(\mathbf{x}_n)$$

  - This is the Delta rule a.k.a. LMS rule!

$\Rightarrow$ Perceptron Learning corresponds to 1st-order (stochastic) Gradient Descent of a quadratic error function!

Loss Functions

- We can now also apply other loss functions
  - L2 loss ⇒ Least-squares regression
    $$L(t, y(\mathbf{x})) = \sum_n \left(y(\mathbf{x}_n) - t_n\right)^2$$
  - L1 loss: ⇒ Median regression
    $$L(t, y(\mathbf{x})) = \sum_n |y(\mathbf{x}_n) - t_n|$$
  - Cross-entropy loss ⇒ Logistic regression
    $$L(t, y(\mathbf{x})) = -\sum_n \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$
  - Hinge loss ⇒ SVM classification
    $$L(t, y(\mathbf{x})) = \sum_n [1 - t_n y(\mathbf{x}_n)]_+$$
  - Softmax loss ⇒ Multi-class probabilistic classification
    $$L(t, y(\mathbf{x})) = -\sum_n \sum_k \left\{ \mathbb{I}(t_n = k) \ln \frac{\exp(y_k(\mathbf{x}))}{\sum_j \exp(y_j(\mathbf{x}))} \right\}$$

Regularization

- In addition, we can apply regularizers
  - E.g., an L2 regularizer

$$E(\mathbf{w}) = \sum_n L(t_n, y(\mathbf{x}_n; \mathbf{w})) + \lambda ||\mathbf{w}||^2$$

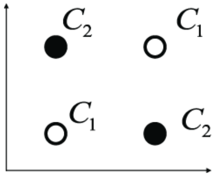
  - This is known as *weight decay* in Neural Networks.
  - We can also apply other regularizers, e.g. L1 $\Rightarrow$ sparsity
  - Since Neural Networks often have many parameters, regularization becomes very important in practice.
  - We will see more complex regularization techniques later on...

Limitations of Perceptrons

- What makes the task difficult?
  - Perceptrons with fixed, hand-coded input features can model any separable function perfectly...
  - ...given the right input features.
  - For some tasks this requires an exponential number of input features.
    - E.g., by enumerating all possible binary input vectors as separate feature units (similar to a look-up table).
    - But this approach won't generalize to unseen test cases!

  ⇒ It is the feature design that solves the task!

  - Once the hand-coded features have been determined, there are very strong limitations on what a perceptron can learn.
    - Classic example: XOR function.



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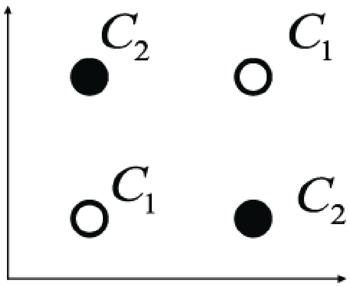
Wait...

- Didn't we just say that...
  - Perceptrons correspond to generalized linear discriminants
  - And Perceptrons are very limited...
  - *Doesn't this mean that what we have been doing so far in this lecture has the same problems???*

- Yes, this is the case.
  - A linear classifier cannot solve certain problems (e.g., XOR).
  - However, with a non-linear classifier based on the right kind of features, the problem becomes solvable.



$\Rightarrow$ So far, we have solved such problems by hand-designing good features ϕ and kernels $\phi^\top\phi$.

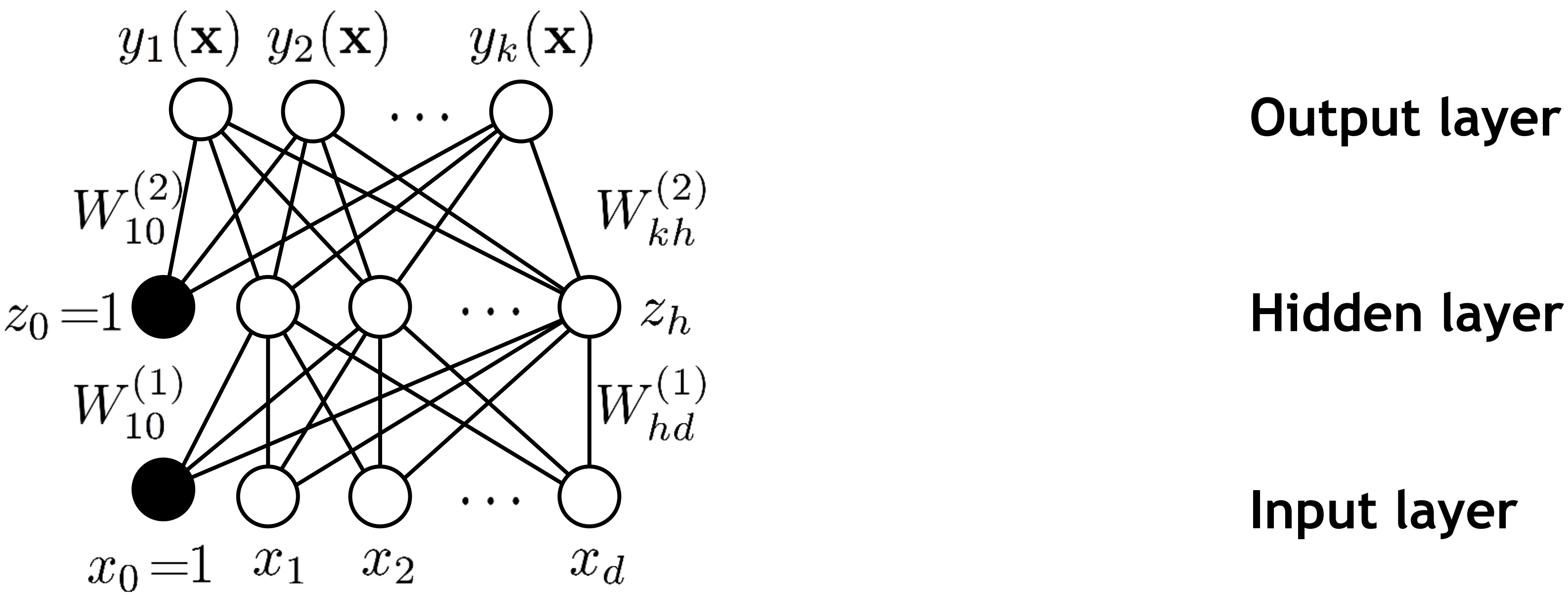
$\Rightarrow$ *Can we also learn such feature representations?*

Topics of This Lecture

- A Short History of Neural Networks
- Perceptrons
  - Definition
  - Loss functions
  - Regularization
  - Limits
- **Multi-Layer Perceptrons**
  - **Definition**
  - **Learning**

Multi-Layer Perceptrons

- **Adding more layers**



- **Output**

$$y_k(\mathbf{x}) = g^{(2)} \left(\sum_{i=0}^{h} W_{ki}^{(2)} g^{(1)} \left(\sum_{j=0}^{d} W_{ij}^{(1)} x_j \right) \right)$$

Multi-Layer Perceptrons

$$y_k(\mathbf{x}) = g^{(2)}\left(\sum_{i=0}^{h} W_{ki}^{(2)} g^{(1)}\left(\sum_{j=0}^{d} W_{ij}^{(1)} x_j\right)\right)$$

- **Activation functions $g^{(k)}$:**
  - **For example:** $g^{(2)}(a) = \sigma(a)$, $g^{(1)}(a) = a$
- **The hidden layer can have an arbitrary number of nodes**
  - **There can also be multiple hidden layers.**
- **Universal approximators**
  - **A 2-layer network (1 hidden layer) can approximate any continuous function of a compact domain arbitrarily well! (assuming sufficient hidden nodes)**

Learning with Hidden Units

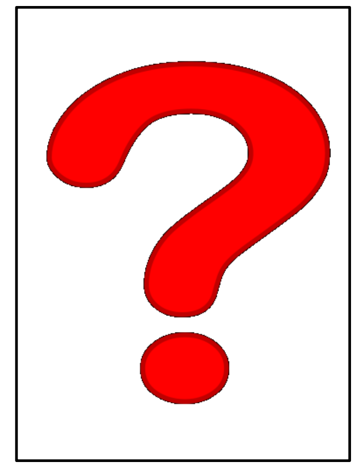
- Networks without hidden units are very limited in what they can learn
  - More layers of linear units do not help ⇒ still linear
  - Fixed output non-linearities are not enough.
- We need multiple layers of adaptive non-linear hidden units. But how can we train such nets?
  - Need an efficient way of adapting all weights, not just the last layer.
  - Learning the weights to the hidden units = learning features
  - This is difficult, because nobody tells us what the hidden units should do.

  ⇒ Next lecture

References and Further Reading

- **More information on Neural Networks can be found in Chapters 6 and 7 of the Goodfellow & Bengio book**

Ian Goodfellow, Aaron Courville, Yoshua Bengio
Deep Learning
MIT Press, in preparation



https://goodfeli.github.io/dlbook/