Advanced Machine Learning
Lecture 12

Neural Networks

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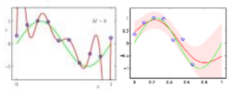
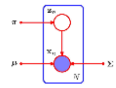
This Lecture: *Advanced Machine Learning*

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

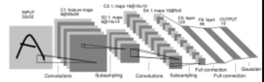
- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Gaussian Processes



- 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

$$y_k(\mathbf{x}) = g\left(\sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})\right) \quad \text{with } \phi_0(\mathbf{x}) = 1$$

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

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

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

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

  - where

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

⇒ Simply feed back the input data point, weighted by the classification error.

Recap: Probabilistic Discriminative Models

- Consider models of the form

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

with

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

- 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

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

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

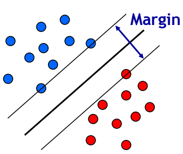
$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} \left\{ \mathbb{I}(t_n = k)\ln \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^{K}\exp(\mathbf{w}_j^\top \mathbf{x})} \right\}$$

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

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"

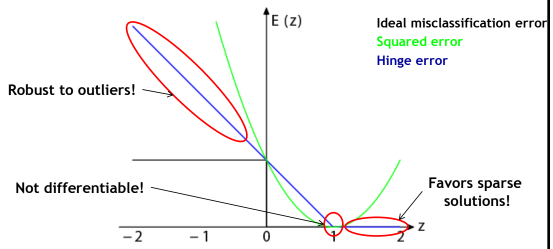
- Different way of looking at it
  - We can reformulate the constraints into the objective function.

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{L_2 \text{ regularizer}} + C\underbrace{\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{"Hinge loss"}}$$

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

Slide adapted from Christoph Lampert

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 ($z_n < 1$).
  - ⇒ Leads to sparse solutions, not sensitive to outliers.
  - Not differentiable around $z_n = 1$ ⇒ Cannot be optimized directly.

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Image source: Bishop, 2006

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SVM - Discussion

- SVM optimization function

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

- 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*

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Topics of This Lecture

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

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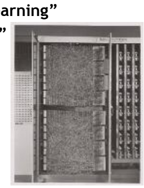
A Brief History of Neural Networks

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."

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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.

Neural Networks don't work!

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Image source: colourbox.de, thinkstock

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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!

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Image sources: clipartpanda.com, cliparts.co

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
- But they are hard to train, tend to overfit, and have unintuitive parameters.
- So, the excitement fades again.

Image source: clipartof.com, colourbox.de

A Brief History of Neural Networks

1957 Rosenblatt invents the Perceptron
1969 Minsky & Papert
1980s Resurgence of Neural Networks
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

1957 Rosenblatt invents the Perceptron
1969 Minsky & Papert
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

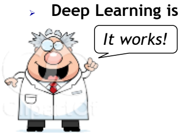
Are you using Neural Networks?

Come on. Get real!

A Brief History of Neural Networks

1957 Rosenblatt invents the Perceptron
1969 Minsky & Papert
1980s Resurgence of Neural Networks
1995+ Interest shifts to other learning methods
2005+ Gradual progress
2012 Breakthrough results

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



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- Perceptrons
  - Definition
  - Loss functions
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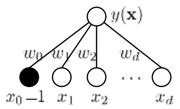
Perceptrons (Rosenblatt 1957)

- **Standard Perceptron**

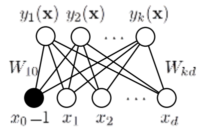


Output layer
Weights
Input layer

- **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 $\mathbf{w}$**

Extension: Multi-Class Networks

- **One output node per class**



Output layer
Weights
Input layer

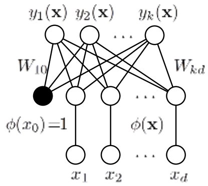
- **Outputs**
  - Linear outputs: $y_k(\mathbf{x}) = \sum_{i=0}^{d} W_{ki} x_i$
  - Logistic outputs: $y_k(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} W_{ki} x_i\right)$

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

Slide adapted from Stefan Roth

Extension: Non-Linear Basis Functions

- **Straightforward generalization**

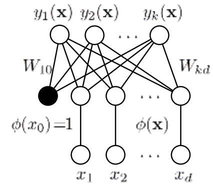


Output layer
Weights
Feature layer
Mapping (fixed)
Input layer

- **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.**

Slide adapted from Geoff Hinton

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**

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

Slide adapted from Geoff Hinton

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!

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

Slide adapted from Geoff Hinton

Loss Functions

- We can now also apply other loss functions
  - L2 loss ⇒ Least-squares regression
    $L(t, y(\mathbf{x})) = \sum_n (y(\mathbf{x}_n) - t_n)^2$
  - 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

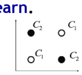
$$E(\mathbf{w}) = \sum_n L(t_n, y(\mathbf{x}_n;\mathbf{w})) + \lambda||\mathbf{w}||^2$$

  - This is known as *weight decay* in Neural Networks.
  - We can also apply other regularizers, e.g. L1 ⇒ 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

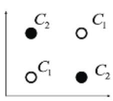
- What makes the task difficult?
  - Perceptrons with fixed, hand-coded input features can model any separable function perfectly...
  - ...given the right input features.
  - For some tasks this requires an exponential number of input features.
    - E.g., by enumerating all possible binary input vectors 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.



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.



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

⇒ *Can we also learn such feature representations?*

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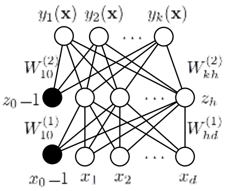
Multi-Layer Perceptrons

- Adding more layers



Output layer

Hidden layer

Input layer

- Output

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

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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)

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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

Slide adapted from Geoff Hinton B. Leibe 41

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/

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