Artificial Intelligence II

Optimization and Neural Nets

[These slides were created by Dan Klein and Pieter Abbeel for CS188 Intro to AI at UC Berkeley. All CS188 materials are available at http://ai.berkeley.edu.]

Lecturer (Hannover): Prof. Dr. Wolfgang Nejdl
Reminder: Linear Classifiers

- Inputs are feature values
- Each feature has a weight
- Sum is the activation

\[ \text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x) \]

- If the activation is:
  - Positive, output +1
  - Negative, output -1
How to get probabilistic decisions?

- **Activation**: \( z = w \cdot f(x) \)
- **If** \( z = w \cdot f(x) \) very positive \( \rightarrow \) want probability going to 1
- **If** \( z = w \cdot f(x) \) very negative \( \rightarrow \) want probability going to 0

- Sigmoid function

\[
\phi(z) = \frac{1}{1 + e^{-z}}
\]
Best $w$?

- Maximum likelihood estimation:

$$\max_w \ ll(w) = \max_w \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

with:

$$P(y^{(i)} = +1|x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

$$P(y^{(i)} = -1|x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

= Logistic Regression
Multiclass Logistic Regression

- Multi-class linear classification
  - A weight vector for each class: \( w_y \)
  - Score (activation) of a class \( y \): \( w_y \cdot f(x) \)
  - Prediction w/highest score wins: \( y = \text{arg max}_y w_y \cdot f(x) \)

- How to make the scores into probabilities?

\[
\begin{align*}
Z_1, Z_2, Z_3 & \rightarrow \frac{e^{Z_1}}{e^{Z_1} + e^{Z_2} + e^{Z_3}}, \quad \frac{e^{Z_2}}{e^{Z_1} + e^{Z_2} + e^{Z_3}}, \quad \frac{e^{Z_3}}{e^{Z_1} + e^{Z_2} + e^{Z_3}}
\end{align*}
\]

original activations \quad softmax activations
Best w?

- Maximum likelihood estimation:

\[
\max_w \ ll(w) = \max_w \sum_i \log P(y^{(i)} | x^{(i)}; w)
\]

with:

\[
P(y^{(i)} | x^{(i)}; w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_y e^{w_y \cdot f(x^{(i)})}}
\]

= Multi-Class Logistic Regression
This Lecture

- Optimization

  i.e., how do we solve:

\[
\max_{w} \quad ll(w) = \max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
\]
Hill Climbing

- Recall from CSPs lecture: simple, general idea
  - Start wherever
  - Repeat: move to the best neighboring state
  - If no neighbors better than current, quit

- What’s particularly tricky when hill-climbing for multiclass logistic regression?
  - Optimization over a continuous space
    - Infinitely many neighbors!
  - How to do this efficiently?
1-D Optimization

- Could evaluate $g(w_0 + h)$ and $g(w_0 - h)$
  - Then step in best direction

- Or, evaluate derivative:
  $$\frac{\partial g(w_0)}{\partial w} = \lim_{h \to 0} \frac{g(w_0 + h) - g(w_0 - h)}{2h}$$
  - Tells which direction to step into
2-D Optimization

Source: offconvex.org
Gradient Ascent

- Perform update in uphill direction for each coordinate
- The steeper the slope (i.e. the higher the derivative) the bigger the step for that coordinate
- E.g., consider: \( g(w_1, w_2) \)

- Updates:

  \[
  w_1 \leftarrow w_1 + \alpha \cdot \frac{\partial g}{\partial w_1}(w_1, w_2)
  \]

  \[
  w_2 \leftarrow w_2 + \alpha \cdot \frac{\partial g}{\partial w_2}(w_1, w_2)
  \]

- Updates in vector notation:

  \[
  w \leftarrow w + \alpha \cdot \nabla_w g(w)
  \]

  with: \( \nabla_w g(w) = \begin{bmatrix}
  \frac{\partial g}{\partial w_1}(w) \\
  \frac{\partial g}{\partial w_2}(w)
  \end{bmatrix} \) = gradient
Gradient Ascent

- Idea:
  - Start somewhere
  - Repeat: Take a step in the gradient direction

Figure source: Mathworks
What is the Steepest Direction?

\[
\max_{\Delta: \Delta_1^2 + \Delta_2^2 \leq \varepsilon} g(w + \Delta)
\]

- **First-Order Taylor Expansion:**
  \[
g(w + \Delta) \approx g(w) + \frac{\partial g}{\partial w_1} \Delta_1 + \frac{\partial g}{\partial w_2} \Delta_2
\]

- **Steepest Descent Direction:**
  \[
  \max_{\Delta: \Delta_1^2 + \Delta_2^2 \leq \varepsilon} g(w) + \frac{\partial g}{\partial w_1} \Delta_1 + \frac{\partial g}{\partial w_2} \Delta_2
  \]

- **Recall:**
  \[
  \max_{\Delta: \|\Delta\| \leq \varepsilon} \Delta^T a \rightarrow \Delta = \varepsilon \frac{a}{\|a\|}
  \]

- **Hence, solution:**
  \[
  \Delta = \varepsilon \frac{\nabla g}{\|\nabla g\|}
  \]

**Gradient direction = steepest direction!**

\[
\nabla g = \left[ \begin{array}{c} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \end{array} \right]
\]
Gradient in n dimensions

\[ \nabla g = \begin{bmatrix}
\frac{\partial g}{\partial w_1} \\
\frac{\partial g}{\partial w_2} \\
\vdots \\
\frac{\partial g}{\partial w_n}
\end{bmatrix} \]
Optimization Procedure: Gradient Ascent

- init $w$
- for iter = 1, 2, ...

$$w \leftarrow w + \alpha \cdot \nabla g(w)$$

- $\alpha$: learning rate --- tweaking parameter that needs to be chosen carefully
- How? Try multiple choices
  - Crude rule of thumb: update changes $w$ about 0.1 – 1%
Batch Gradient Ascent on the Log Likelihood Objective

\[
\max_w \ ll(w) = \max_w \sum_i \log P(y^{(i)}|x^{(i)}; w)
\]

\[g(w)\]

- init \( w \)
- for iter = 1, 2, ...
  \[w \leftarrow w + \alpha \sum_i \nabla \log P(y^{(i)}|x^{(i)}; w)\]
Stochastic Gradient Ascent on the Log Likelihood Objective

$$\max_w \ ll(w) = \max_w \ \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

**Observation:** once gradient on one training example has been computed, might as well incorporate before computing next one

- **init** $w$
- **for** iter = 1, 2, ...
  - **pick** random j
  $$w \leftarrow w + \alpha \cdot \nabla \log P(y^{(j)}|x^{(j)}; w)$$
Mini-Batch Gradient Ascent on the Log Likelihood Objective

\[
\max_w \ ll(w) = \max_w \sum_i \log P(y^{(i)} | x^{(i)}; w)
\]

**Observation:** gradient over small set of training examples (=mini-batch) can be computed in parallel, might as well do that instead of a single one

- **init** \( w \)
- **for** iter = 1, 2, ...
  - pick random subset of training examples \( J \)
  \[
  w \leftarrow w + \alpha \sum_{j \in J} \nabla \log P(y^{(j)} | x^{(j)}; w)
  \]
How about computing all the derivatives?

- We’ll talk about that once we covered neural networks, which are a generalization of logistic regression
Multi-class Logistic Regression

- = special case of neural network

\[ P(y_1|x; w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}} \]
\[ P(y_2|x; w) = \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}} \]
\[ P(y_3|x; w) = \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}} \]
Deep Neural Network = Also learn the features!

\[ P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}} \]
\[ P(y_2|x;w) = \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}} \]
\[ P(y_3|x;w) = \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}} \]
Deep Neural Network = Also learn the features!

\[ z_i^{(k)} = g\left( \sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)} \right) \]

\( g = \text{nonlinear activation function} \)
Deep Neural Network = Also learn the features!

\[ z_i^{(k)} = g \left( \sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)} \right) \]

\[ g = \text{nonlinear activation function} \]
Common Activation Functions

**Sigmoid Function**

\[ g(z) = \frac{1}{1 + e^{-z}} \]

\[ g'(z) = g(z)(1 - g(z)) \]

**Hyperbolic Tangent**

\[ g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \]

\[ g'(z) = 1 - g(z)^2 \]

**Rectified Linear Unit (ReLU)**

\[ g(z) = \max(0, z) \]

\[ g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases} \]
Training the deep neural network is just like logistic regression:

\[
\max_{w} \quad ll(w) = \max_{w} \sum_{i} \log P(y^{(i)}|x^{(i)}; w)
\]

just \( w \) tends to be a much, much larger vector 😊

→ just run gradient ascent

+ stop when log likelihood of hold-out data starts to decrease
Theorem (Universal Function Approximators). A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.

Practical considerations

- Can be seen as learning the features
- Large number of neurons
  - Danger for overfitting
  - (hence early stopping!)
Universal Function Approximation Theorem*

**Hornik theorem 1:** Whenever the activation function is bounded and nonconstant, then, for any finite measure $\mu$, standard multilayer feedforward networks can approximate any function in $L^p(\mu)$ (the space of all functions on $\mathbb{R}^k$ such that $\int_{\mathbb{R}^k} |f(x)|^p d\mu(x) < \infty$) arbitrarily well, provided that sufficiently many hidden units are available.

**Hornik theorem 2:** Whenever the activation function is continuous, bounded and non-constant, then, for arbitrary compact subsets $X \subseteq \mathbb{R}^k$, standard multilayer feedforward networks can approximate any continuous function on $X$ arbitrarily well with respect to uniform distance, provided that sufficiently many hidden units are available.

- **In words:** Given any continuous function $f(x)$, if a 2-layer neural network has enough hidden units, then there is a choice of weights that allow it to closely approximate $f(x)$.

Cybenko (1989) “Approximations by superpositions of sigmoidal functions”
Hornik (1991) “Approximation Capabilities of Multilayer Feedforward Networks”
Leshno and Schocken (1991) “Multilayer Feedforward Networks with Non-Polynomial Activation Functions Can Approximate Any Function”
Universal Function Approximation Theorem*

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Fun Neural Net Demo Site

- Demo-site:
  - http://playground.tensorflow.org/
How about computing all the derivatives?

- Derivatives tables:

\[
\begin{align*}
\frac{d}{dx}(a) &= 0 \\
\frac{d}{dx}(x) &= 1 \\
\frac{d}{dx}(au) &= a \frac{du}{dx} \\
\frac{d}{dx}(u + v - w) &= \frac{du}{dx} + \frac{dv}{dx} - \frac{dw}{dx} \\
\frac{d}{dx}(uv) &= u \frac{dv}{dx} + v \frac{du}{dx} \\
\frac{d}{dx}\left(\frac{u}{v}\right) &= \frac{1}{v} \frac{du}{dx} - \frac{u}{v^2} \frac{dv}{dx} \\
\frac{d}{dx}(u^n) &= nu^{n-1} \frac{du}{dx} \\
\frac{d}{dx}(\sqrt{u}) &= \frac{1}{2\sqrt{u}} \frac{du}{dx} \\
\frac{d}{dx}\left(\frac{1}{u}\right) &= -\frac{1}{u^2} \frac{du}{dx} \\
\frac{d}{dx}\left(\frac{1}{u^n}\right) &= -\frac{n}{u^{n+1}} \frac{du}{dx} \\
\frac{d}{dx}[f(u)] &= \frac{d}{du}[f(u)] \frac{du}{dx} \\
\frac{d}{dx}[\ln u] &= \frac{d}{dx}[\log_e u] = \frac{1}{u} \frac{du}{dx} \\
\frac{d}{dx}[\log_a u] &= \log_a e \frac{1}{u} \frac{du}{dx} \\
\frac{d}{dx}[e^n] &= e^n \frac{du}{dx} \\
\frac{d}{dx}[a^u] &= a^u \ln a \frac{du}{dx} \\
\frac{d}{dx}[u^v] &= vu^{v-1} \frac{du}{dx} + \ln u \ u^v \frac{dv}{dx} \\
\frac{d}{dx}[\sin u] &= \cos u \frac{du}{dx} \\
\frac{d}{dx}[\cos u] &= -\sin u \frac{du}{dx} \\
\frac{d}{dx}[\tan u] &= \sec^2 u \frac{du}{dx} \\
\frac{d}{dx}[\cot u] &= -\csc^2 u \frac{du}{dx} \\
\frac{d}{dx}[\sec u] &= \sec u \tan u \frac{du}{dx} \\
\frac{d}{dx}[\csc u] &= -\csc u \cot u \frac{du}{dx}
\end{align*}
\]

[source: http://hyperphysics.phy-astr.gsu.edu/hbase/Math/derfunc.html]
How about computing all the derivatives?

- But neural net $f$ is never one of those?
  - No problem: CHAIN RULE:

  If \[ f(x) = g(h(x)) \]

  Then \[ f'(x) = g'(h(x))h'(x) \]

→ Derivatives can be computed by following well-defined procedures
Automatic Differentiation

- Automatic differentiation software
  - e.g. Theano, TensorFlow, PyTorch, Chainer
  - Only need to program the function \( g(x,y,w) \)
  - Can automatically compute all derivatives w.r.t. all entries in \( w \)
  - This is typically done by caching info during forward computation pass of \( f \), and then doing a backward pass = “backpropagation”
  - Autodiff / Backpropagation can often be done at computational cost comparable to the forward pass
- Need to know this exists
- How this is done? -- outside of scope of CS188
Summary of Key Ideas

- Optimize probability of label given input
  \[ \max_w ll(w) = \max_w \sum_i \log P(y^{(i)}|x^{(i)}; w) \]

- Continuous optimization
  - Gradient ascent:
    - Compute steepest uphill direction = gradient (= just vector of partial derivatives)
    - Take step in the gradient direction
    - Repeat (until held-out data accuracy starts to drop = “early stopping”)

- Deep neural nets
  - Last layer = still logistic regression
  - Now also many more layers before this last layer
    - = computing the features
    - → the features are learned rather than hand-designed
  - Universal function approximation theorem
    - If neural net is large enough
    - Then neural net can represent any continuous mapping from input to output with arbitrary accuracy
    - But remember: need to avoid overfitting / memorizing the training data → early stopping!
  - Automatic differentiation gives the derivatives efficiently (how? = outside of scope of 188)
How well does it work?
Computer Vision
Object Detection
Manual Feature Design
Features and Generalization

[HoG: Dalal and Triggs, 2005]
Features and Generalization

Image

HoG
Performance

ImageNet Error Rate 2010-2014

Error Rate

79% 60% 40% 20% 7%

2010 2011 2012 2013 2014

Traditional CV

graph credit Matt Zeiler, Clarifai
Performance

ImageNet Error Rate 2010-2014

- Traditional CV
- Deep Learning

Error Rate

- 79%
- 60%
- 40%
- 20%
- 7%


AlexNet

Graph credit Matt Zeiler, Clarifai
Performance

ImageNet Error Rate 2010-2014

- Traditional CV
- Deep Learning

Graph credit: Matt Zeiler, Clarifai
Performance

ImageNet Error Rate 2010-2014

- Traditional CV
- Deep Learning

AlexNet

Error Rate

graph credit Matt Zeiler, Clarifai
MS COCO Image Captioning Challenge

"man in black shirt is playing guitar."

"construction worker in orange safety vest is working on road."

"two young girls are playing with lego toy."

"boy is doing backflip on wakeboard."

"girl in pink dress is jumping in air."

"black and white dog jumps over bar."

"young girl in pink shirt is swinging on swing."

"man in blue wetsuit is surfing on wave."

Karpathy & Fei-Fei, 2015; Donahue et al., 2015; Xu et al, 2015; many more
Visual QA Challenge
Stanislaw Antol, Aishwarya Agrawal, Jiasen Lu, Margaret Mitchell, Dhruv Batra, C. Lawrence Zitnick, Devi Parikh

What vegetable is on the plate?
Neural Net: broccoli
Ground Truth: broccoli

What color are the shoes on the person's feet?
Neural Net: brown
Ground Truth: brown

How many school busses are there?
Neural Net: 2
Ground Truth: 2

What sport is this?
Neural Net: baseball
Ground Truth: baseball

What is on top of the refrigerator?
Neural Net: magnets
Ground Truth: cereal

What uniform is she wearing?
Neural Net: shorts
Ground Truth: girl scout

What is the table number?
Neural Net: 4
Ground Truth: 40

What are people sitting under in the back?
Neural Net: bench
Ground Truth: tent
Speech Recognition

TIMIT Speech Recognition

graph credit Matt Zeiler, Clarifai
Machine Translation

Google Neural Machine Translation (in production)
Next: More Neural Net Applications!