Topics:

- Linear Classification, Loss functions
- Gradient Descent

CS 4644-DL / 7643-A ZSOLT KIRA

• Assignment 1 out last week!

- Start early, start early, start early!
- HW1 Tutorial: <u>https://piazza.com/class/ky0k0ha5vgy1mk?cid=41</u>
- **Piazza:** Enroll now! <u>https://piazza.com/gatech/spring2022/cs46447643a</u> (Code: DLSPR2022)
 - **NOTE:** There is an OMSCS section with a Ed. Make sure you are in the right one
- Office hours schedule:

https://piazza.com/class/ky0k0ha5vgy1mk?cid=40

Parametric Model

Explicitly model the function $f : X \rightarrow Y$ in the form of a parametrized function f(x, W) = y, **examples**:

Logistic regression/classification

Neural networks

Capacity (size of hypothesis class) **does not** grow with size of training data!

Learning is **search**

Supervised Learning

Parametric – Linear Classifier

$$f(x,W) = Wx + b$$

Procedure:

Calculate score per class for example Return label of maximum score (argmax)





Components of a Parametric Model



- Input: Continuous number or vector
- **Output:** A continuous number
 - For classification typically a **score**
 - For regression what we want to regress to (house prices, crime rate, etc.)
 - *w* is a vector and weights to optimize to fit target function

Model: Discriminative Parameterized Function





Deep Learning as Legos

Georg

- Idea: Separate classes via high-dimensional linear separators (hyper-planes)
- One of the simplest parametric models, but surprisingly effective
 - Very commonly used!
- Let's look more closely at each element



Linear Classification and Regression



To simplify notation we will refer to inputs as $x_1 \cdots x_m$ where $m = n \times n$

Input Dimensionality



(Note that in practice, implementations can use xW instead, assuming a different shape for W. That is just a different convention and is equivalent.)



- We can move the bias term into the weight matrix, and a "1" at the end of the input
- Results in one matrix-vector multiplication!

Model f(x, W) = Wx + b

 $\begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} & b_1 \\ w_{21} & w_{22} & \cdots & w_{2m} & b_2 \\ w_{31} & w_{32} & \cdots & w_{3m} & b_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \\ 1 \end{bmatrix}$





Example with an image with 4 pixels, and 3 classes (cat/dog/ship)



Stretch pixels into column

Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n





Visual Viewpoint

We can convert the weight vector back into the shape of the image and visualize



Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n





Geometric Viewpoint

 $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{W}) = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$



Array of **32x32x3** numbers (3072 numbers total)

Plot created using Wolfram Cloud

Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n





Class 1: number of pixels > 0 odd Class 2: number of pixels > 0 even







Class 1: Three modes Class 2: Everything else



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Performance Measure for a Classifier





Components of a Parametric Model

- The output of a classifier can be considered a score
- For binary classifier, use rule:

 $y = \begin{cases} 1 & \text{if } f(x, w) > = 0 \\ 0 & \text{otherwise} \end{cases}$

- Can be used for many classes by considering one class versus all the rest (one versus all)
- For multi-class classifier can take the maximum



Classification using Scores

Several issues with scores:

- Not very interpretable (no bounded value)
- We often want probabilities
- More interpretable
- Can relate to probabilistic view of machine learning

We use the **softmax** function to convert scores to probabilities

$$s = f(x, W)$$
 Scores

$$P(Y = k | X = x) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$
 Softmax
Function



We need a performance measure to **optimize**

- Penalizes model for being wrong
- Allows us to modify the model to reduce this penalty
- Known as an objective or loss function

In machine learning we use **empirical risk minimization**

- Reduce the loss over the training dataset
- We average the loss over the training data

Given a dataset of examples:

 $\{(x_i, y_i)\}_{i=1}^N$

Where x_i is image and y_i is (integer) label

Loss over the dataset is a sum of loss over examples:

 $L = \frac{1}{N} \sum L_1(f(x_i, W), y_i)$





Given an example $(x_{i,}y_{i})$ where x_{i} is the image and where y_{i} is the (integer) label,



and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_{i} = \sum_{j \neq y_{i}} \begin{cases} 0 & \text{if } s_{y_{i}} \geq s_{j} + \\ s_{j} - s_{y_{i}} + 1 & \text{otherwise} \end{cases}$$
$$= \sum_{j \neq y_{i}} max(0, s_{j} - s_{y_{i}} + 1)$$



Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n

Performance Measure for Scores

1

Given an example $(x_{i,}y_{i})$ where x_{i} is the image and where y_{i} is the (integer) label,

and using the shorthand for the scores vector: $s = f(x_i, W)$

 $max(0, s_j - s_{y_i} + 1)$

the SVM loss has the form:

 $= \max(0, 5.1 - 3.2 + 1)$

 $+\max(0, -1.7 - 3.2 + 1)$

 $= \max(0, 2.9) + \max(0, -3.9)$

 $L_i =$

= 2.9 + 0

= 2.9

Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:



Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n

SVM Loss Example



Given an example $(x_{i,}y_{i})$ where x_{i} is the image and where y_{i} is the (integer) label,

and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form: $L_{i} = \sum_{j \neq y_{i}} max(0, s_{j} - s_{y_{i}} + 1)$ = max(0, 1.3 - 4.9 + 1) + max(0, 2.0 - 4.9 + 1) = max(0, -2.6) + max(0, -1.9) = 0 + 0 Cat

= 0

Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:



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SVM Loss Example

 $L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$

Q: What happens to loss if car image scores change a bit?

No change for small values

Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:



3.21.32.25.14.92.5-1.72.0-3.1

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cat

car

frog

Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:

$$L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$$

Q: What is min/max of loss value?

[0,inf]



cat	3.2	1.3	2.2
car	5.1	4.9	2.5
frog	-1.7	2.0	-3.1

Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n



 $L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$

Q: At initialization W is small so all $s \approx 0$. What is the loss?

C-1

Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:



cat	3.2	1.3	2.2
car	5.1	4.9	2.5
rog	-1.7	2.0	-3.1

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 $L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$

Q: What if the sum was over all classes? (including j = y_i)

No difference (add constant 1)

Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:



cat	3.2	1.3	2.2
car	5.1	4.9	2.5
frog	-1.7	2.0	-3.1

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 $L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$

Q: What if we used mean instead of sum?

No difference Scaling by constant Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:



cat	3.2	1.3	2.2
car	5.1	4.9	2.5
frog	-1.7	2.0	-3.1

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Given an example $(x_{i,}y_{i})$ where x_{i} is the image and where y_{i} is the (integer) label,

and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$$

L = (2.9 + 0 + 12.9)/3 = **5.27** Suppose: 3 training examples, 3 classes. With some *W* the scores f(x,W)=Wx are:



cat	3.2	1.3	2.2
car	5.1	4.9	2.5
frog	-1.7	2.0	-3.1
osses:	2.9	0	12.9

Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n

SVM Loss Example



$$egin{aligned} f(x,W) &= Wx \ L &= rac{1}{N} \sum_{i=1}^N \sum_{j
eq y_i} \max(0, f(x_i;W)_j - f(x_i;W)_{y_i} + 1) \end{aligned}$$

E.g. Suppose that we found a W such that L = 0. Q: Is this W unique?

No 2W also has L=0

Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n



- If we use the softmax function to convert scores to probabilities, the right loss function to use is cross-entropy
- Can be derived by looking at the distance between two probability distributions (output of model and ground truth)
- Can also be derived from a maximum likelihood estimation perspective

s = f(x, W) Scores

 $P(Y = k | X = x) = \frac{e^{s_k}}{\sum_j e^{s_j}}$ Softmax Function

$$L_i = -\log P(Y = y_i | X = x_i)$$

Maximize log-prob of correct class = Maximize the log likelihood = Minimize the negative log likelihood

Performance Measure for Probabilities

- If we use the softmax function to convert scores to probabilities, the right loss function to use is cross-entropy
- Goal: Minimize KL-divergence (distance measure b/w probability distributions)

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$$p^{*} = \begin{bmatrix} 0\\0\\0\\1\\0\\0\\0\\0\\0\\0\\0\end{bmatrix} \qquad \hat{p} = \begin{bmatrix} P(Y = 1 | x, w)\\P(Y = 2 | x, w)\\P(Y = 3 | x, w)\\P(Y = 3 | x, w)\\P(Y = 4 | x, w)\\P(Y = 5 | x, w)\\P(Y = 6 | x, w)\\P(Y = 6 | x, w)\\P(Y = 7 | x, w)\\P(Y = 8 | x, w)\end{bmatrix} = \begin{bmatrix} 0.5\\0.01\\0.01\\0.01\\0.01\\0.15\\0.3\end{bmatrix}$$

Prediction

Ground Truth

$$\begin{split} \min_{w} KL(p^*||\hat{p}) &= \sum_{y} p^*(y) \log \frac{p^*(y)}{\hat{p}(y)} \\ &= \sum_{y} p^*(y) \log(p^*(y)) - \sum_{y} p^*(y) \log(\hat{p}(y)) \\ &\stackrel{-H(p^*)}{\text{(negative entropy, term goes away)}} \sum_{y} H(p^*, \hat{p}) \\ & \text{(Cross-Entropy)} \end{split}$$

parameters we are minimizing over)

Since p^* is one-hot (0 for non-ground truth classes), all we need to minimize is (where *i* is ground truth class): min $(-\log \hat{p}(y_i))$

Performance Measure for Probabilities

Softmax Classifier (Multinomial Logistic Regression)



Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n

Cross-Entropy Loss Example

Softmax Classifier (Multinomial Logistic Regression)



Want to interpret raw classifier scores as **probabilities**



Probabilities must be >= 0



Q: What is the min/max of possible loss L_i?

Infimum is 0, max is unbounded (inf)

Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n



Cross-Entropy Loss Example

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as probabilities



Probabilities must be >= 0



Q: At initialization all s will be approximately equal; what is the loss?

Log(C), e.g. $log(10) \approx 2$

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Cross-Entropy Loss Example



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Cross-Entropy Loss Example

If we are performing **regression**, we can directly optimize to match the ground truth value

Example: House price prediction

 $L_i = |y - W x_i| \qquad \mathsf{L1}$

 $L_i = |y - W x_i|^2 \qquad L2$



Source: https://raw.githubusercontent.com/rohanvarma/rohan-blog/gh-pages/images/loss3.jpg



Often, we add a regularization term to the loss function

L1 Regularization

$$L_i = |y - Wx_i|^2 + |W|$$

Example regularizations:

L1/L2 on weights (encourage small values)





Gradient Descent





Components of a Parametric Model

Given a model and loss function, finding the best set of weights is a **search problem**

 Find the best combination of weights that minimizes our loss function

Several classes of methods:

- Random search
- Genetic algorithms (population-based search)
- Gradient-based optimization

In deep learning, **gradient-based methods are dominant** although not the only approach possible



Optimization

As weights change, the loss changes as well

 This is often somewhatsmooth locally, so small changes in weights produce small changes in the loss

We can therefore think about iterative algorithms that take current values of weights and modify them a bit







We can find the steepest descent direction by computing the derivative (gradient):

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

- Steepest descent direction is the negative gradient
- Intuitively: Measures how the function changes as the argument a changes by a small step size
 - As step size goes to zero
- In Machine Learning: Want to know how the loss function changes as weights are varied
 - Can consider each parameter separately by taking partial derivative of loss function with respect to that parameter







This idea can be turned into an algorithm (gradient descent)

• Choose a model:
$$f(x, W) = Wx$$

Choose loss function: $L_i = |y - Wx_i|^2$

Calculate partial derivative for each parameter: $\frac{\partial L}{\partial w_i}$

• Update the parameters:
$$w_i = w_i - \frac{\partial L}{\partial w_i}$$

• Add learning rate to prevent too big of a step: $w_i = w_i - \alpha \frac{\partial L}{\partial w_i}$

Repeat (from Step 3)

Gradient Descent



http://demonstrations.wolfram.com/VisualizingTheGradientVector/









Often, we only compute the gradients across a small subset of data

Full Batch Gradient Descent

$$L = \frac{1}{N} \sum L\left(f(x_i, W), y_i\right)$$

Mini-Batch Gradient Descent

$$L = \frac{1}{M} \sum L(f(x_i, W), y_i)$$

- Where M is a *subset* of data
- We iterate over mini-batches:
 - Get mini-batch, compute loss, compute derivatives, and take a set





Gradient descent is guaranteed to converge under some conditions

- For example, learning rate has to be appropriately reduced throughout training
- It will converge to a *local* minima
 - Small changes in weights would not decrease the loss
- It turns out that some of the local minima that it finds in practice (if trained well) are still pretty good!



Gradient Descent Properties

We know how to compute the **model output and loss function**

Several ways to compute $\frac{\partial L}{\partial w_i}$

- Manual differentiation
- Symbolic differentiation
- Numerical differentiation
- Automatic differentiation



Computing Gradients





current W:	W + h (first dim):	gradient dW:
[0.34,	[0.34 + 0.0001 ,	[?,
-1.11,	-1.11,	?,
0.78,	0.78, 0.12	?,
0.55,	0.55,	?.
2.81,	2.81,	?,
-3.1,	-3.1,	?,
-1.5,	-1.5,	?,
0.33,]	0.33,]	?,]
loss 1.25347	loss 1.25322	

current W:	W + h (first dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,]	[0.34 + 0.0001 , -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,] Ioss 1.25322	$[-2.5, ?, ?, ?, ?, ?, ?, ?, ?, ?, ?,]$ $(1.25322 - 1.25347)/0.0001 = -2.5$ $\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$?, ?,]

current W:	W + h (second dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12,	[0.34, -1.11 + 0.0001 , 0.78, 0.12,	[-2.5, ?, ?, ?,
0.55, 2.81	0.55, 2.81.	?,
-3.1, -1.5,	-3.1, -1.5,	?, ?, ?.
0.33,…] loss 1.25347	0.33,…] loss 1.25353	?,]

current W:	W + h (second dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12,	[0.34, -1.11 + 0.0001 , 0.78, 0.12,	[-2.5, 0.6, ▶ ?, ?, ?,
0.55, 2.81, -3.1, -1.5,	0.55, 2.81, -3.1, -1.5,	(1.25353 - 1.25347)/0.0001 = 0.6 $\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$
0.33,…] loss 1.25347	0.33,…] Ioss 1.25353	?,]

current W:	W + h (third dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12, 0.55	[0.34, -1.11, 0.78 + 0.0001 , 0.12, 0.55	[-2.5, 0.6, ?, ?,
0.55, 2.81, -3.1, -1.5,	0.55, 2.81, -3.1, -1.5,	?, ?, ?, ?, ?,
0.33,…] loss 1.25347	0.33,…] loss 1.25347	?,]



Numerical vs Analytic Gradients

$$rac{df(x)}{dx} = \lim_{h o 0} rac{f(x+h) - f(x)}{h}$$

Numerical gradient: slow :(, approximate :(, easy to write :) **Analytic gradient**: fast :), exact :), error-prone :(

In practice: Derive analytic gradient, check your implementation with numerical gradient. This is called a **gradient check.**

- Components of parametric classifiers:
 - Input/Output: Image/Label
 - Model (function): Linear Classifier + Softmax
 - Loss function: Cross-Entropy
 - Optimizer: Gradient Descent
- Ways to compute gradients
 - Numerical
 - Next: Analytical, automatic differentiation





For some functions, we can analytically derive the partial derivative

Example:

FunctionLoss $f(w, x_i) = w^T x_i$ $(y_i - w^T x_i)^2$

(Assume w and \mathbf{x}_i are column vectors, so same as $w \cdot x_i$)

Update Rule $w_j \leftarrow w_j + 2\eta \sum_{k=1}^N \delta_k x_{kj}$

Derivation of Update Rule

Manual Differentiation