CS 4644 / 7643-A DEEP LEARNING: LECTURE 3 DANFEI XU

- Linear Classifier (cont.)
- SVM / Hinge Loss
- Softmax Classifier and Cross-Entropy Loss
- Gradient Descent

Machine Learning Applications



MISC

- Make sure you know how to use Google Colab
- PS1 release 08/29
- Use Piazza!
- Start to find your project team!
- Shared sample project report in @6 on Piazza.





Recap:

Supervised Learning

- Train Input: {*X*, *Y*}
- Learning output: f: $X \rightarrow Y$, e.g. P(y|x)

- Unsupervised Learning
- Input: {X}

• Learning output: P(x)

Example: Clustering, density estimation, etc.

Reinforcement Learning

- Supervision in form of reward
- No supervision on what action to take

Very often combined, sometimes within the same model!











Recap:



This time:

f(x, W) = Wx



airplane	-3.45	-0.51	3.42
automobile	-8.87	6.04	4.64
bird	0.09	5.31	2.65
cat	2.9	-4.22	5.1
deer	4.48	-4.19	2.64
dog	8.02	3.58	5.55
frog	3.78	4.49	-4.34
horse	1.06	-4.37	-1.5
ship	-0.36	-2.09	-4.79
truck	-0.72	-2.93	6.14

1.Define a **loss function** that quantifies our unhappiness with the scores across the training data.

2. Come up with a way of efficiently finding the parameters that minimize the loss function. **(optimization)**

Loss Function and Optimization



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



cat car frog **3.2**1.35.1**4.9**-1.72.0

High Loss Low Loss

2.5 **-3.1**

2.2

oss High Loss

A **loss function** that tells how good the current classifier is

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:

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





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: $s_i = f(x_i, W)$

the SVM loss has the form:

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

Notation: s_{y_i} is the **score** given by the classifier for the correct label class of the i-th example (y_i)

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: $s = f(x_i, W)$

the SVM loss has the form:

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



Performance Measure for Scores



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: $s = f(x_i, W)$

= 2.9

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



3.2 1.3 2.2 cat the SVM loss has the form: $\max(0, s_j - s_{y_i} + 1)$ 5.1 2.5 4.9 $L_i =$ car -1.7 2.0 -3.1 $= \max(0, 5.1 - 3.2 + 1) +$ frog max(0, -1.7 - 3.2 + 1)2.9 Losses: $= \max(0, 2.9) + \max(0, -3.9)$ = 2.9 + 0





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

= 0

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







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: $L_i = \sum_{j \neq v_i} max(0, s_j - s_{y_i} + 1)$ L = (2.9 + 0 + 12.9)/3.osses: = 5.27

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



3.2	1.3	2.2
5.1	4.9	2.5
-1.7	2.0	-3.1
2.9	0	12.9

Adapted from from CS 231n slides



cat

car

frog



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

Q: What happens to loss if car image scores change a bit (e.g., \pm 0.1)?

No change for small values

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



Adapted from from CS 231n slides



cat

car

frog

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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 from CS 231n slides



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

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

num_class - 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

Adapted from from CS 231n slides



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

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

Q: What if we used mean instead of sum?



	cat	3.2	1.3	2.2
No difference	car	5.1	4.9	2.5
Scaling by constant	frog	-1.7	2.0	-3.1

Adapted from from CS 231n slides



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

```
def hinge_loss_vec(x, y, W):
    """
    x (d): input example vectors
    y (int): class label
    W (C x d): weight matrix
    """
    scores = W.dot(x)  # calculate raw scores
    margins = np.maximum(0, scores - scores[y] + 1) # calculate margins s_j - s_{yi} + 1
    margins[y] = 0 # exclude yi from the loss sum
    loss_i = np.sum(margins). # sum across all j (classes)
    return loss_i
```





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

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

Let's look at an example





cat

car

frog

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



Before:

 $= \max(0, 1.3 - 4.9 + 1)$ $+ \max(0, 2.0 - 4.9 + 1)$ $= \max(0, -2.6) + \max(0, -1.9)$ = 0 + 0= 0

With W twice as large: = max(0, 2.6 - 9.8 + 1)+max(0, 4.0 - 9.8 + 1)= max(0, -6.2) + max(0, -4.8)= 0 + 0= 0





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

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

No, 2W also has L=0 How do we choose between W, 2W, and 1e+7W?





Regularization intuition: fitting a polynomial function







Regularization intuition: fitting a polynomial function f_2 y Train Data Χ

Adapted from from CS 231n slides



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Regularization intuition: fitting a polynomial function







Regularization

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data





Reference: https://icml.cc/Conferences/2004/proceedings/papers/354.pdf

. .

Regularization

 λ = regularization strength (hyperparameter)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing too well on training data

Simple examples L2 regularization: $R(W) = \sum_{k} \sum_{l} W_{k,l}^2$ L1 regularization: $R(W) = \sum_{k} \sum_{l} |W_{k,l}|$

More complex (DNN-specific): Dropout

Stochastic depth, fractional pooling, etc

Batch/layer normalization

Elastic net (L1 + L2): $R(W) = \sum_{k} \sum_{l} \beta W_{k,l}^{2} + |W_{k,l}|$

Regularization

Regularization: Implement a simple L2 regularizer

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

```
def l2_regularized_hinge_loss(x, y, W, reg_coeff):
    data_loss = 0
    # calculate dataset loss
    for i in range(x.shape[0]):
        data_loss += hinge_loss_vec(x[i], y[i], W)
```

```
# calculate weight regularization loss
reg_loss = np.sum(np.square(W)) * reg_coeff
```

```
return data_loss + reg_loss
```





What if we want probabilities?



*Technically we can get probability from SVM classifiers too, see Platt scaling

Performance Measure using Probabilities











3.2

5.1

-1.7

Unnormalized log-

probabilities / logits

softmax

cat

car

frog

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

$$s = f(x_i; \theta)$$

0.13

0.87

0.00

Predicted

Probs

(softmax)

$$p_{\theta}(\mathbf{Y} = \mathbf{y}_i | \mathbf{X} = \mathbf{x}_i) = \frac{e^{s_{y_i}}}{\sum_j e^{s_j}}$$
 Sof

Softmax Function

We maximize the probability of $p_{\theta}(y_i|x_i)!$

Finding a set of weights θ that maximizes the probability of correct prediction: $\underset{\theta}{\operatorname{argmax}} \prod p_{\theta}(y_i|x_i)$ This is equivalent to:

$$\operatorname{argmax}_{\theta} \sum \ln p_{\theta}(y_i | x_i)$$
$$L_i = -\ln p_{\theta}(y_i | x_i) = -\ln \left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right) = -\ln(0.13)$$

1. Maximum Likelihood Estimation (MLE): Choose weights to maximize the likelihood of observed data. In this case, the loss function is the **Negative Log-Likelihood (NLL)**.





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

$$s = f(x_i; \theta)$$

$$p_{\theta}(Y = y_i | X = x_i) = \frac{e^{s_{y_i}}}{\sum_j e^{s_j}}$$
 Softmax Function

We maximize the probability of $p_{\theta}(y_i|x_i)!$

cat 3.2 car 5.1 frog -1.7 Unnormalized logprobabilities / logits for (softmax) Finding a set of weights θ that maximizes the probability of correct prediction: $\underset{\theta}{\operatorname{argmax}} \prod p_{\theta}(y_i|x_i)$ This is equivalent to:

$$\operatorname{argmax}_{\theta} \sum \ln p_{\theta}(y_i | x_i)$$

$$L_i = -\ln p_{\theta}(y_i | x_i) = -\ln \left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right) = -\ln(0.13)$$
Negative Log Likelihood (NLL)







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





NLL and CrossEntropy are different loss functions in PyTorch!

CROSSENTROPYLOSS

CLASS torch.nn.CrossEntropyLoss(weight=None, size_average=None, ignore_index=- 100, reduce=None, reduction='mean', label_smoothing=0.0) [SOURCE] Expects unformalized logits as input (the function will apply softmax & log on top)

NLLLOSS

Expects log probabilities as input (do softmax yourself!)







Want to interpret raw classifier scores as probabilities

 $s = f(x_i; \theta)$

$$p_{\theta}(\boldsymbol{Y} = \boldsymbol{y}_i | \boldsymbol{X} = \boldsymbol{x}_i) = \frac{\boldsymbol{e}^{s_{y_i}}}{\sum_j \boldsymbol{e}^{s_j}}$$

Softmax Function

Cross-entropy loss:

$$L_i = -\log(p_\theta(y_i|x_i))$$

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

Infimum is 0, max is unbounded (inf)



Want to interpret raw classifier scores as probabilities

 $s = f(x_i; \theta)$

$$p_{\theta}(\mathbf{Y} = \mathbf{y}_i | \mathbf{X} = \mathbf{x}_i) = \frac{e^{s_{y_i}}}{\sum_j e^{s_j}}$$

Softmax Function

Cross-entropy loss:

$$L_i = -\log(p_\theta(y_i|x_i))$$

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

 $-\log(1/C)$, e.g. $-\log(1/3) = \log(3) \approx 1.1$





Use logistic function as example. Same as general softmax but for binary classification

$$\sigma(x) = \frac{e^x}{1 + e^x}$$

Consider the following three basis for NLL:

- 1. Squash and clip network value (x) to (0, 1]
- 2. (Negative) logistic function
- 3. NLL with logistic function







Use logistic function as example. Same as general softmax but for binary classification

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- 3. NLL with logistic function

Softmax is a normalization function that behaves well with Cross Entropy Loss.

3. NLL w/ logistic: Strong guidance when classifier is wrong



So, what is a loss function?

- In this context, it's a function that scores how well a **model** performs on a task. We often focus on the parameters rather than the hypothesis class.
- If $L(\theta_1, data) < L(\theta_2, data)$, then θ_1 is considered better.
- Losses are different than metrics. Loss functions are designed for optimization, which require properties like differentiability and smoothness.
- Example: CrossEntropy is a loss function for the multi-class classification task. Classification accuracy (how often the model is correct) is the metric.
- Losses can be used as metrics but are often not very interpretable.
- Losses can always be used as metrics, but metrics often cannot be used as loss functions (e.g., classification accuracy is not differentiable).

Summary: SVM and Softmax Classifier

- Loss function: performance measure to improve
 - Find weights that better satisfies the objective
- Multiclass SVM Classifier
 - Predicts class score
 - Hinge loss: "maximum margin" objective: $L_i = \sum_{j \neq y_i} max(0, s_j s_{y_i} + 1)$
- Regularization
 - Prevent overly complex function that only works well on the training set
- Softmax Classifier
 - Predicts class probabilities
 - To train softmax classifiers: use NLL and Cross Entropy Loss







- Functional form of the model
 - Including parameters
- Performance measure to improve
 - Loss or objective function
- Algorithm for finding best parameters

Data: Image

Optimization algorithm





Strategy #1: A first very bad idea solution: Random search

```
# assume X train is the data where each column is an example (e.g. 3073 x 50,000)
# assume Y train are the labels (e.g. 1D array of 50,000)
# assume the function L evaluates the loss function
bestloss = float("inf") # Python assigns the highest possible float value
for num in xrange(1000):
  W = np.random.randn(10, 3073) * 0.0001 # generate random parameters
  loss = L(X train, Y train, W) # get the loss over the entire training set
  if loss < bestloss: # keep track of the best solution
    bestloss = loss
    bestW = W
  print 'in attempt %d the loss was %f, best %f' % (num, loss, bestloss)
# prints:
# in attempt 0 the loss was 9.401632, best 9.401632
# in attempt 1 the loss was 8.959668, best 8.959668
# in attempt 2 the loss was 9.044034, best 8.959668
# in attempt 3 the loss was 9.278948, best 8.959668
# in attempt 4 the loss was 8.857370, best 8.857370
# in attempt 5 the loss was 8.943151, best 8.857370
# in attempt 6 the loss was 8.605604, best 8.605604
# ... (trunctated: continues for 1000 lines)
```

Optimization



Lets see how well this works on the test set...

Assume X_test is [3073 x 10000], Y_test [10000 x 1]
scores = Wbest.dot(Xte_cols) # 10 x 10000, the class scores for all test examples
find the index with max score in each column (the predicted class)
Yte_predict = np.argmax(scores, axis = 0)
and calculate accuracy (fraction of predictions that are correct)
np.mean(Yte_predict == Yte)
returns 0.1555

15.5% accuracy! not bad! (SOTA is ~99.7%) Adapted from from CS 231n slides





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



- Calculate the gradients of a loss function with respect to a set of parameters (w's).
- Update the parameters towards the gradient direction that minimizes the loss.





Gradient Descent: Follow the Slope!

0



As weights change, the gradients change 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**:

 $\frac{\partial f}{\partial w} = \lim_{h \to 0} \frac{f(w+h) - f(w)}{h}$

- **Gradient** is multi-dimensional derivatives
- Notation: $\frac{\partial f}{\partial w}$ is the gradient of f(e.g., a loss function)with respect to variable w (e.g., a weight vector).
- $\frac{\partial f}{\partial w}$ is of the **same shape** as w
- Intuitively: Measures how the *output* changes as the variable w changes by a small step size
- Steepest descent direction is the negative gradient
- Gradient descent: Minimize loss by changing parameters







current W:	gradient dW:
[0.34,	[?,
-1.11,	?,
0.78,	?.
0.12,	?.
0.55,	?.
2.81,	?
-3.1,	?.
-1.5,	?
0.33,]	?]
loss 1.25347	.,

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

current W:	W + h (first dim):
[0.34,	[0.34 + 0.0001 ,
-1.11,	-1.11,
0.78,	0.78,
0.12,	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

gradient dW:

[?,

?,

?,

?,

?,

?, ?,

?,

?,...]

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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



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

gradient dW:

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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 , ?,
0.12, 0.55, 2.81, -3.1,	0.12, 0.55, 2.81, -3.1,	(1.25353 - 1.25347)/0.0001 = 0.6 $\frac{df(x)}{dx} = \lim_{x \to 0} \frac{f(x+h) - f(x)}{h}$
-1.5, 0.33,…] loss 1.25347	│ -1.5, │ 0.33,…] │ Ioss 1.25353	$?,\ldots]$

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

current W:	W + h (third dim):	
[0.34,	[0.34,	
-1.11,	-1.11,	
0.78,	0.78 + 0.0001 ,	
0.12,	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 1.25347	

gradient dW:

[-2.5, 0.6, ?, ?, ?, ?, ?, ?, ?,...]

W + h (third dim):
[0.34,
-1.11,
0.78 + 0.0001 ,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,]
loss 1.25347



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

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

More on autodiff:

https://www.cs.toronto.edu/~rgrosse/courses/csc421_201 9/readings/L06%20Automatic%20Differentiation.pdf



Computing Gradients



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 implement Analytic gradient: fast, exact, error-prone (if implemented from scratch)

Almost all differentiable functions that you can think of have analytical gradients implemented in popular libraries, e.g., PyTorch, TensorFlow.

If you want to derive your own gradients, check your implementation with numerical gradient. This is called a **gradient check**.

The gradient descent algorithm

- 1. Choose a model: f(x, W) = Wx
- 2. Choose loss function: $L_i = |y Wx_i|^2$
- 3. Calculate partial derivative for each parameter: $\frac{\partial L}{\partial w_i}$
- 4. Update the parameters: $w_i = w_i \frac{\partial L}{\partial w_i}$
- 5. Add learning rate to prevent too big of a step: $w_i = w_i \alpha \frac{\partial L}{\partial w_i}$

Repeat 3-5





Composing simple functions creates complex analytical gradients



Adapted from slides by: Marc'Aurelio Ranzato, Yann LeCun







∂L _	∂L	∂p	ди
$\frac{\partial w}{\partial w}$	$\overline{\partial p}$	$\overline{\partial u}$	∂w

Next time: Chain rule and Backpropagation!

Adapted from slides by: Marc'Aurelio Ranzato, Yann LeCun



