Machine Learning: Linear Classification & Optimization

ROB 102: Introduction to AI & Programming

Lecture 12

2021/11/29

Project 4: Machine Learning

Implement three machine learning algorithms to classify images from the MNIST dataset.

- 1. Nearest neighbors
- 2. Linear Classifier (Today!)
- 3. Neural Network

Last time...

We saw the (k-)Nearest Neighbor algorithm.

We assumed an image is numerically close to other images in the same class.

distance(λ , λ)

At training time, we saved ALL our training data, and calculated distances at test time.



Summary: Nearest Neighbors

Pros:

- + Straight-forward to implement
- + No training necessary
- + "Pretty good" for many problems

Cons:

- Requires a lot of memory
- Expensive at test time
- Distance isn't always a good indicator of class similarity
- We need many training examples to make a good classifier for high dimensions (like images!)

Class Scores

What if we had a function that told us how "two-like" an image is?

$$f_2(2) = \text{score}$$

The score should be HIGH the image is a two and LOW if the image is probably not a two.

Most modern machine learning algorithms do classification like this.



Now, we only need to learn the parameters of a function using our training data. We don't need to save the training data anymore.

Image



Recall: Machine Learning Algorithm

Training time:

Find a function f(X) which does well at classifying training data.

Testing time: Use f(X) to classify new data.

Recall: Machine Learning Algorithm

Training time:

Find a function f(X) which does well at classifying labelled data.

Testing time: Use f(X) to classify new data.

How do we choose what f(X) should look like?

How do we learn f(X)?

Recall: Machine Learning Algorithm

Training time:

Find a function f(X) which does well at classifying labelled data.

Testing time: Use f(X) to classify new data.

How do we choose what f(X) should look like? \succ Next: Use a linear function

Let's look at a 2-D example. We want to classify our points into two categories:



We need a function, f(X) which will help us find a label, y_{pred} , which is 1 if the image is of a two, and -1 if it is not a two.





What does this look like in code? Remember, our plan is to use a linear function. In 1-D, this looks like this:



Images as Vectors

We will rearrange our images into long vectors by flattening them. The vectors will have length W*H.



For MNIST images, vectors will have length 28*28 = 784.

For our image, with dimension D = 28*28:

$$f(X) = w^{(1)}x^{(1)} + w^{(2)}x^{(2)} + \dots + w^{(D-1)}x^{(D-1)} + w^{(D)}x^{(D)} + b$$



Dot Product

A convenient way of writing this is called the dot product of vectors:

$$f(X) = W \cdot X + b$$

$$\uparrow$$
Dot product



 $= w^{(1)}x^{(1)} + w^{(2)}x^{(2)} + \dots + w^{(D)}x^{(D)} + b$

Example: Dot Product



Example: Dot Product



 $= 0.2 \cdot 56 + -0.5 \cdot 231 + 0.1 \cdot 24 + 2.0 \cdot 2 + 1.1$

= -96.8

Let's go back and take a look at our choice of model, f(X). What does it mean to use a linear model?

$f(X) = W \cdot X + b$

If we can draw a straight line through our data, then we say it is <u>linearly</u> <u>separable</u>.



If we can draw a straight line through our data, then we say it is <u>linearly</u> <u>separable</u>.



Linear classifier assumption: The data is linearly separable.

The problem with assumptions...



"All models are wrong, but some models are useful."

Translation: Let's assume our linear model is "good enough"

Multiple Classes

In MNIST we have 10 classes, so we learn 10 classifiers (10 weight vectors).

Each classifier gives a score for a class. We predict that the image belongs to the class that gives it the highest score.



Multiple Classes

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Multiple Classes

If we have K classes, we can find K linear functions (K weight vectors and biases):

$$f_1(X) = W_1 \cdot X + b_1$$
$$f_2(X) = W_2 \cdot X + b_2$$
$$\vdots$$
$$f_K(X) = W_K \cdot X + b_K$$

Linear Classifier Algorithm

Training: Find weights *W* and bias *b* that do well at classifying training data

Testing: For each class *i*, do: $f_i(X) = W_i \cdot X + b_i$

Assign label: $y_{pred} = \underset{i}{\operatorname{argmax}} f_i(X)$



airplane	-3.45	-0.51	3.42
automobile	-8.87	<i>Ypred</i> 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 <i>Ypred</i>	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	<i>Ypred</i> 6.14

Matrix Multiplication

For the multiple class case, we need to perform *K* dot products between the weight vectors and images.



Matrix multiplication allows us to do this operation in one step.

Matrix Multiplication



Matrix multiplication takes the dot product between each row of the first matrix with each column of the second matrix.

Example: Matrix Multiplication



Image:

Parameters:















Matrix Multiplication in Julia

```
julia> W = [0.2 -0.5 0.1 2; -0.2 0 0.4 1.3; 1.1 -0.7 0.6 -0.2]
3×4 Matrix{Float64}:
 0.2 -0.5 0.1 2.0
 -0.2 0.0 0.4 1.3
 1.1 -0.7 0.6 -0.2
julia> X = [56; 231; 24; 2]
4-element Vector{Int64}:
 56
231
 24
  2
julia> b = [1.1; -0.3; 0.9]
3-element Vector{Float64}:
 1.1
 -0.3
 0.9
 ulia>
```

julia> W * X
3-element Vector{Float64}:
 -97.89999999999999
 1.0
 -86.09999999999998

julia> W * X + b
3-element Vector{Float64}:
 -96.8
 0.7
 -85.199999999999997

julia>

The * operation between two matrices is a matrix multiplication in Julia.
Project 4: Matrix Multiplication



Note: This will give us the same answer, $X \cdot W_i$ with instead of $W_i \cdot X$. Project 4 uses this representation (images stacked in rows).

Matrix Shapes

We write matrix shape as: #rows x #columns Or: (rows, columns)





Matrix Multiplication in Julia

juli	ia>/	A =	[1	23	; 4	5	6;	7	8	9;	10	11	12]
4×3	Mati	rix	{Int	:64}	:								_
1	2		3	-									
4	5	(5										
7	8	9	9										
10	11	12	2										
juli (4,	ia> 9 3)	size	≥(A))									
juli 3×2	ia> I Matı	3 = rix:	[3 {Int	3; t64}	22	;	1 1]					
3	3												
2	2												
1	1												
juli	ia> s	size	≥(B))									
(3,	2)												
juli	ia≻												

julia> A * B
4×2 Matrix{Int64}:
10 10
28 28
46 46
64 64
julia> size(A * B) (4, 2)
julia>

Legal!

The inner dimensions match:

 $(4, 3) \times (3, 2) \rightarrow (4, 2)$

Matrix Multiplication in Julia

jul:	ia> A	= [1	L 2 3	; 4	5	6;	7	8	9;	10	11	12
4×3	Matr	ix{Ir	nt64}	:								
1	2	3	-									
4	5	6										
7	8	9										
10	11	12										
jul: (4,	ia> s 3)	ize(#	4)									
jul	ia> B	= [3	33;	2 2	;	1 1]					
3×2	Matr	ix{Ir	1t64}	:								
3	3											
2	2											
1	1											
jul	ia≻ s	ize(E	3)									
(3,	2)											
jul:	ia≻											



We get the same answer if we do dot products between the rows of A and the columns of B!

Matrix Multiplication in Julia

iuli	a> A	= [1	2	3:	4	5	6:	7	8	9:	10	11	12
4×3	Matr	ix{In	t64	4}:			-,			- ,			
1	2	3											
4	5	6											
7	8	9											
10	11	12											
juli	a> s	ize(A)										
(4,	(4, 3)												
juli	julia> C = [1 1 1; 2 2 2]												
2x2 Matnix(Int64).													

2x3 Matrix{Int64}: 1 1 1 2 2 2 2 julia> size(C) (2, 3)

julia> A * C

ERROR: DimensionMismatch("matrix A has dimension
s (4,3), matrix B has dimensions (2,3)")
Stacktrace:

[1] _generic_matmatmul!(C::Matrix{Int64}, tA::C har, tB::Char, A::Matrix{Int64}, B::Matrix{Int64} }, _add::LinearAlgebra.MulAddMul{true, true, Boo l, Bool})

@ LinearAlgebra C:\buildbot\worker\package_wi
n64\build\usr\share\julia\stdlib\v1.6\LinearAlge
bra\src\matmul.jl:814

Illegal 😕

The inner dimensions don't match:

 $(4, 3) \times (2, 3) \rightarrow Fails!$

One more trick...



One more trick...



**but (D+1) x K parameters

Images as Matrices

When we have multiple images, we will stack them up into a big matrix. For N images, the matrix will have size Nx(W*H).



MNIST has 60,000 training images. The training image matrix will have size 60,000x784.

Training the model

How do we find **W**?

 $f(X) = X \times W$

We will use optimization!

Gradient Descent Optimization

An optimization algorithm helps us find the best *local* (lowest or highest) value of a function.

We will use an algorithm called **gradient descent** to find the weights.

First, we need something to optimize.



How can we train a linear classifier?



Which of these classifiers is better?

Recall: Overfitting

We would like our model to perform well on new data, even if that sacrifices performance on training data.

How can we train a linear classifier?



Idea: We want to find a function which maximizes a margin.

This will make our algorithm more stable to perturbations in the input.

We might misclassify an example or two in our training set, but hopefully we'll get a function which is better at classifying new images.

Loss Function

A loss function tells us how good a model is at classifying an image.

The loss is **LOW** if we're doing a good job at classifying, and **HIGH** if we're doing a bad job.

Our goal is to find weights W that *minimize* the loss. This is called optimization. (More on that later).

Support Vector Machine (SVM) Loss

Idea: The score for the correct class of an image should be higher than the other scores by some margin.

Aside: Why is it called "support vector machine"?



SVM Loss

Goal: Images should be classified correctly by at least a margin Δ .

Say for some image X, its correct label is y with score $f_y(X)$. For all classes $i \neq y$, we want:

Incorrect class score

$$\underset{\text{score}}{\text{Correct class}} \to f_y(X) \ge f_i(X) + \Delta$$

In other words, the score for some incorrect class, $f_i(X)$ is less than the correct class score by at least Δ .

SVM Loss

If the margin condition is met, then we're happy! We will set $L_i = 0$. Otherwise, the loss will be the amount by which we are off:

Incorrect class score
$$L_i = (f_i(X) + \Delta) - f_y(X) \leftarrow Correct class score score$$

The total loss is the sum of the losses for each class that is not correct:

$$L = \sum_{\forall i \setminus y} \begin{cases} f_i(X) + \Delta - f_y(X) & \text{if } f_y(X) < f_i(X) + \Delta \\ 0 & \text{otherwise} \end{cases}$$

Note: $\forall i \setminus y$ means "for all values of i except y"

SVM Loss

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Incorrect class score
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In English: For each incorrect class, add its loss to the total, if it wasn't less than the correct class by the margin.

$$L_{i} = \begin{cases} f_{i}(X) + \Delta - f_{y}(X) & \text{if } f_{y}(X) < f_{i}(X) + \Delta \\ 0 & \text{otherwise} \end{cases}$$
SVM LOSS

Example: SVM Loss



Exercise: Find the SVM Loss for each image.

classes

Example: SVM Loss
$$L_i = \begin{cases} f_i(X) + \Delta - f_y(X) & \text{if } f_y(X) < f_i(X) + \Delta \\ 0 & \text{otherwise} \end{cases}$$

					Exercise: Find the SVM Loss for each image.				
	A.S.	(555)			$\Delta = 1$				
				car:	5.1 + 1 = 6.1 > 3.2				
cat	3.2	1.3	2.2		$L_{car} = 6.1 - 3.2 = 2.9$				
car	5.1	4.9	2.5	frog:	-1.7 + 1 = -0.7 < 3.2				
frog	-1.7	2.0	-3.1		$L_{frog} = 0$				
	29			L = 2	<mark>.9 + 0 =</mark> 2.9				

Example: SVM Loss
$$L_i = \begin{cases} f_i(X) + \Delta - f_y(X) & \text{if } f_y(X) < f_i(X) + \Delta \\ 0 & \text{otherwise} \end{cases}$$



Example: SVM Loss
$$L_i = \begin{cases} f_i(X) + \Delta - f_y(X) & \text{if } f_y(X) < f_i(X) + \Delta \\ 0 & \text{otherwise} \end{cases}$$

cat	3.2	1.3	2.2	C
car	5.1	4.9	2.5	
rog	-1.7	2.0	-3.1	
	2.9	0	12.9 mage Credit: Johnson (link)	

Exercise: Find the SVM Loss for each image. $\Delta = 1$ cat: 2.2 + 1 = 3.2 > -3.1 $L_{cat} = 3.2 - -3.1 = 6.3$ car: 2.5 + 1 = 3.5 > -3.1 $L_{frog} = 3.5 - -3.1 = 6.6$ L = 6.3 + 6.6 = 12.9

$$L_{i} = \begin{cases} f_{i}(X) + \Delta - f_{y}(X) & \text{if } f_{y}(X) < f_{i}(X) + \Delta \\ 0 & \text{otherwise} \end{cases}$$

Example: SVM Loss



Exercise: Find the SVM Loss for each image. $\Delta = 1$

Total Loss: = (2.9 + 0 + 12.9) / 3 = 5.27

How can we train a linear classifier?

Goal: Find a set of weights *W* that minimizes the loss.

Idea #1: Random Search

- 1. Set weights randomly
- 2. Check how well the classifier does



Idea #1: Random Search

- 1. Set weights randomly
- 2. Check how well the classifier does



Idea #1: Random Search

- 1. Set weights randomly
- 2. Check how well the classifier does



Idea #1: Random Search

Until we're happy with the performance, do:

- 1. Set weights randomly
- 2. Check how well the classifier does

Bad idea! We have 785x10 different numbers to find. This will take forever.



Imagine you're hiking (blindfolded!). You want to get to the lowest point of the hill.

Idea:

- 1. Try to take a step.
- 2. Stay there if you get lower than your current location.
- 3. Repeat!



Idea #2: Random Local Search

Set the weights randomly

- 1. Take a small step in a random direction
- 2. If the loss improves, update the weights



Idea #2: Random Local Search

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- 1. Take a small step in a random direction
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Idea #2: Random Local Search

Set the weights randomly

Until we're happy with the performance, do:

- 1. Take a small step in a random direction
- 2. If the loss improves, update the weights

Better, but still not great. It will be hard to find the right direction to step.



Rate of Change

Can we do better?

Yes! With Calculus 🙂


Rate of Change

The slope at a point is given by:

slope = $\frac{\Delta y}{\Delta x}$

This is the rate of change of y. It tells us how y changes if we change x a little.



Rate of Change

The slope at a point is given by:

rate of change
$$=\frac{\Delta y}{\Delta x}$$

Recall from calculus:

$$\int \frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x}$$
gradient



Gradient

Recall from calculus:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x}$$

In 2D, the gradient is the direction and rate of fastest increase.

gradients in 2D
$$\rightarrow \begin{bmatrix} \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2} \end{bmatrix}$$

partial derivatives





Gradient

Recall from calculus:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x}$$

In 2D, the gradient is the direction and rate of fastest increase.

gradients in 2D
$$\rightarrow \left[\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}\right]$$



Idea: We can use the gradient of the loss function to figure out how to update our weights!

Idea #3: Following the gradient

Set the weights randomly

Until we're happy with the performance, do:



Idea #3: Following the gradient

Set the weights randomly

Until we're happy with the performance, do:



Idea #3: Following the gradient

Set the weights randomly

Until we're happy with the performance, do:



Idea #3: Following the gradient

Set the weights randomly

Until we're happy with the performance, do:



Idea #3: Following the gradient

Set the weights randomly

Until we're happy with the performance, do:



Idea #3: Following the gradient

Set the weights randomly

Until we're happy with the performance, do:

1. Take a small step in the direction of the gradient

Better! And we can compute the gradients ahead of time because we know how to do the derivatives.



Gradient descent algorithm:

W = random_normal(D, K) * eps
for iteration in 1:N do:
 loss_grad = SVM_grad(SVM_loss, X, W)
 W = W - step_size * loss_grad

Gradient descent algorithm:

Gradient descent algorithm:

of

Gradient descent algorithm:



Gradient descent algorithm:



Update the weight in the opposite direction of the gradient

Gradient is the direction of maximum *increase*, and we want the loss to *decrease*, so we use the *negative* of the gradient.

Gradient descent algorithm:



Update the weight in the opposite direction of the gradient

How do we calculate the gradient?

How do we pick the step size?

Computing the Gradient

We can take the gradient of the loss with respect to each weight:

$$\frac{\partial L}{\partial W} = \begin{bmatrix} \frac{\partial L}{\partial w_1^{(1)}} & \cdots & \frac{\partial L}{\partial w_K^{(1)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial L}{\partial w_1^{(D)}} & \cdots & \frac{\partial L}{\partial w_K^{(D)}} \end{bmatrix}$$

The gradient of the loss with respect to the weights is a matrix with the same size as the weights (D x K).

Computing the Gradient

We can take the gradient of the loss with respect to each weight:

$$\frac{\partial L}{\partial W} = \begin{bmatrix} \frac{\partial L}{\partial w_1^{(1)}} & \cdots & \frac{\partial L}{\partial w_K^{(1)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial L}{\partial w_1^{(D)}} & \cdots & \frac{\partial L}{\partial w_K^{(D)}} \end{bmatrix}$$

We know the loss function, so we can compute the gradient beforehand. You are given a function to compute the gradients in P4!

Computing the Gradient

You are given a function to compute the gradients in P4!

If you want to derive them, check out the notes for Stanford course CS231n. (link)

$$egin{aligned}
abla_{w_{y_i}}L_i &= -\left(\sum_{j
eq y_i} 1(w_j^Tx_i - w_{y_i}^Tx_i + \Delta > 0)
ight)x_i \
abla_{w_j}L_i &= 1(w_j^Tx_i - w_{y_i}^Tx_i + \Delta > 0)x_i \end{aligned}$$

Computing the Gradient in Julia

The provided gradient function is called in the function that computes the loss

```
function svm_loss(W, X, y, reg=0)
# Grab useful constants.
N, D = size(X)
_, C = size(W)
loss = 0.0
delta = 1
# Get all the scores (NxC).
scores = linear_forward(W, X)
# TODO: Calculate the scores, then calculate the loss. Don't forget
# the regularization term in the loss function!
dW = linear_svm_grad(W, X, y, scores, reg) 	This function computes gradients
return loss, dW
end
```

Gradient descent algorithm:



Update the weight in the opposite direction of the gradient

How do we calculate the gradient?

How do we pick the step size?

Learning Rate

The step size, which tells us how big of a step to take along the gradient, is called the learning rate.

If we take a huge step, we might overshoot, and get farther away from the minimum.



Learning Rate

N, = size(X)

losses = zeros(num iters) for it in 1:num iters

The step size, which tells us how big of a step to take along the gradient, is called the learning rate.

If we take a small step, it will take a long time to find good weights.

The learning rate is a hyperparameter we need to set!

Learning rate



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Mini-Batch Gradient Descent

Gradient descent algorithm:



Mini-Batch Gradient Descent

Instead of computing the loss for every single training image at every iteration (expensive!!) we will only compute loss for a small randomly selected **batch** of data.

We will assume that this gives us a reasonable estimate of what the loss would look like over all the data.

In P4.2, your functions should accept batches of image data, instead of one image. The image matrix X will have shape (N, D) where N is batch size.

Regularization

Let's say we have a set of weights which classify all the images with 100% accuracy.

$$f(X) = W \times X$$

Any scalar multiplication of the weight matrix will also classify the images perfectly. There are infinite of these matrices!!

$$f(X) = \alpha W \times X$$

That's going to make it hard to find good weights.

Regularization

The solution to this is to add an additional part to our loss function which tries to classify images correctly while <u>keeping the weights small</u>.

We'll add a regularization loss to the overall loss function:

$$L_{reg}(W) = \alpha \sum_{i=1}^{D} \sum_{j=1}^{K} \left(w_{j}^{(i)} \right)^{2}$$
Regularization
coefficient
(need to tune this)
$$\sum_{i=1}^{N} \sum_{j=1}^{K} \left(w_{j}^{(i)} \right)^{2}$$
Sum of all the squared weights
in the weight matrix

Regularization

The solution to this is to add an additional part to our loss function which tries to classify images correctly while <u>keeping the weights small</u>.

We'll add a regularization loss to the overall loss function:

$$L_{reg}(W) = \alpha \sum_{i=1}^{D} \sum_{j=1}^{K} \left(w_{j}^{(i)} \right)^{2}$$

$$L(X, W, y) = L_{SVM}(W, X, y) + L_{reg}(W)$$

Tuning Hyperparameters

Play with the parameters in the notebook!



Maybe even try implementing a validation fold or cross validation to find reg and lr.

Tuning Hyperparameters

The loss curve is a plot of loss over time. It's a good way to check your machine learning algorithm is learning.



Tuning Hyperparameters

You can also look at the training and validation accuracies to see how your training is going



```
P4.2: Linear classifiers
```

```
function train_svm(W, X, y, num_classes, lr=0.01, reg=1e-3, batch=20, num_iters=100, print_freq=100)
N, _ = size(X)
losses = zeros(num_iters)
for it in 1:num_iters
# TODO: Sample a random batch of size `batch`, get the loss
# and gradient, and update the weights. Remember to save the
# loss in the losses vector at `losses[it]`.

if it % print_freq == 0
println("Iteration ", it, ": average loss = ", sum(losses) / it)
end
end
return losses, W
end
```

Next time: Neural networks!