Topics:

- Linear Classification, Loss functions
- Gradient Descent

CS 4644-DL / 7643-A ZSOLT KIRA

Assignment 1 out!

- Due Feb. 3rd
- Start early, start early, start early!
- HW1 Tutorial: Monday
- Matrix Calculus Tutorial: next Thursday
- Piazza: Enroll now! (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/lcl94yjxkbb59e/post/59

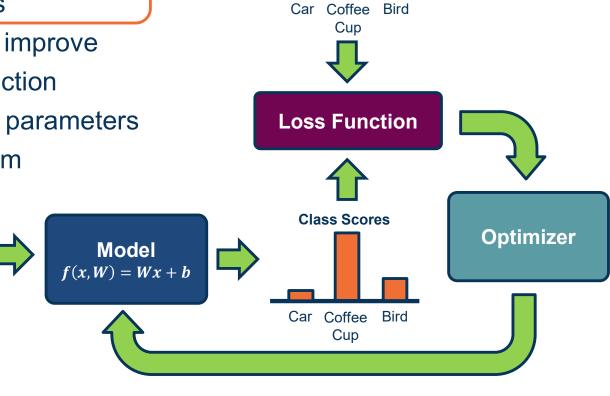
Use canvas zoom schedule



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

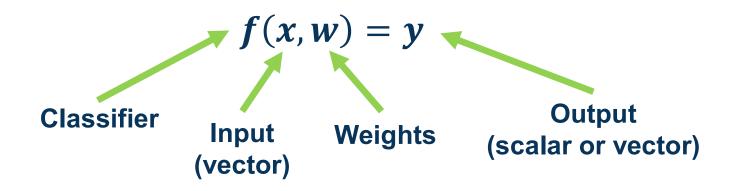


Data: Image



Class Scores





- 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



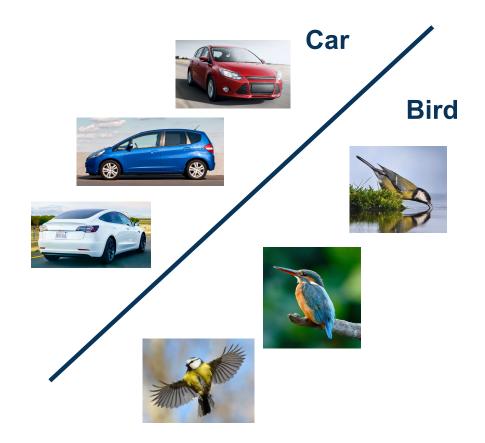
Neural Network



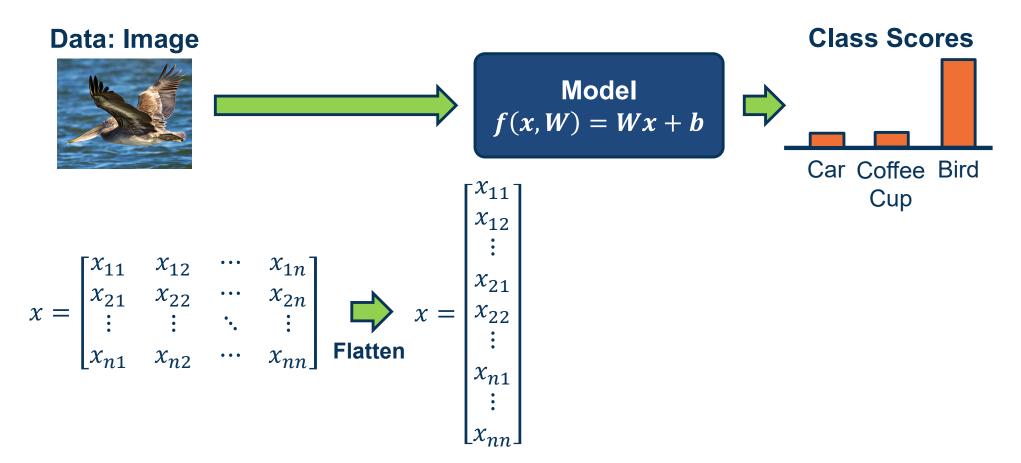
Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n



- 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







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



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

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

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

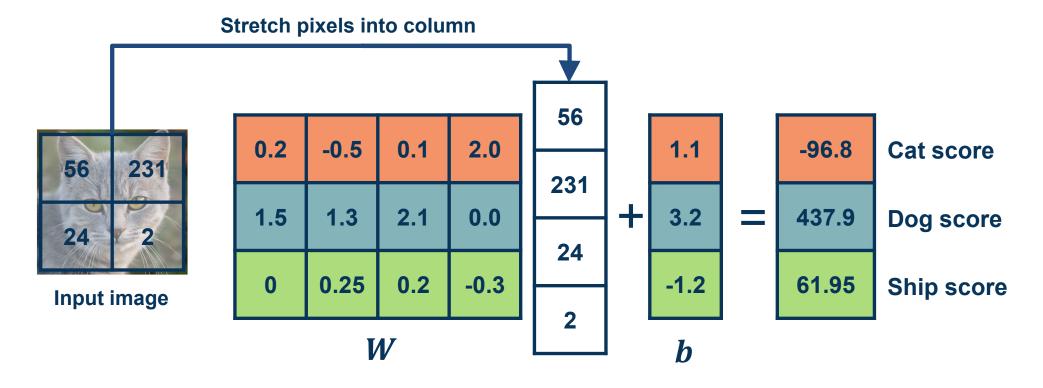


- We can move
 the bias term
 into the weight
 matrix, and a "1"
 at the end of the
 input
- Results in one matrix-vector multiplication!

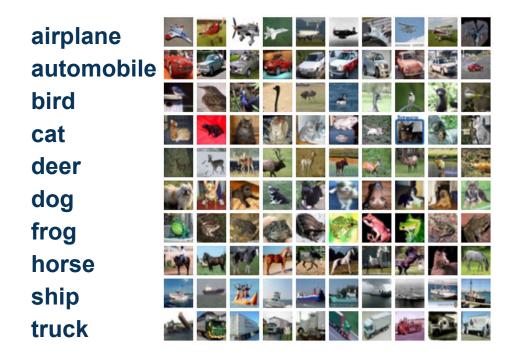
Modelf(x, W) = Wx + b

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

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





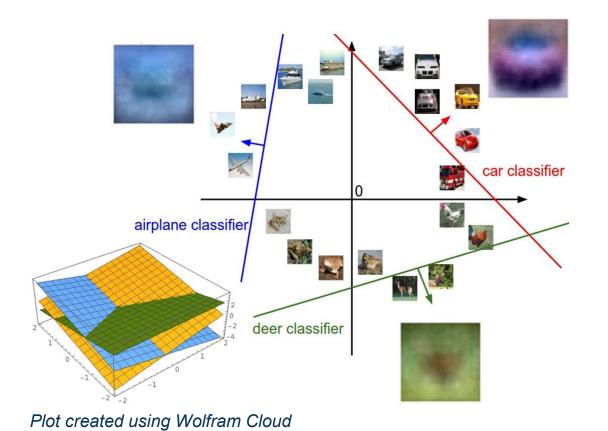


Visual Viewpoint

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







Geometric Viewpoint

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



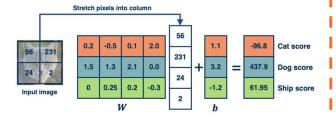
Array of **32x32x3** numbers (3072 numbers total)

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

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Algebraic Viewpoint

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



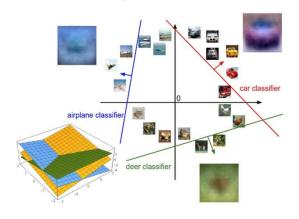
Visual Viewpoint

One template per class



Geometric Viewpoint

Hyperplanes cutting up space

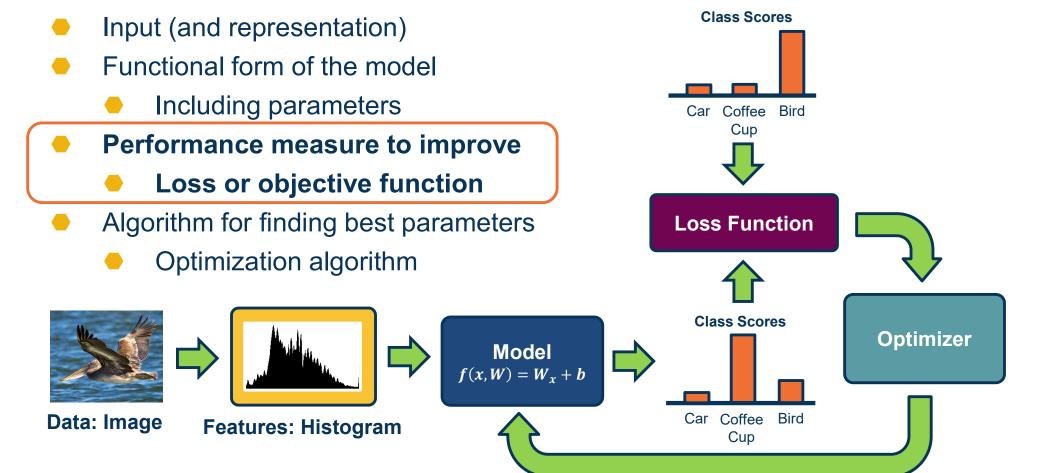


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Performance Measure for a Classifier



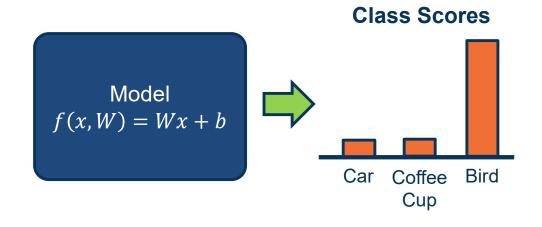




- The output of a classifier can be considered a score
- For binary classifier, use rule:

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

- 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





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:

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

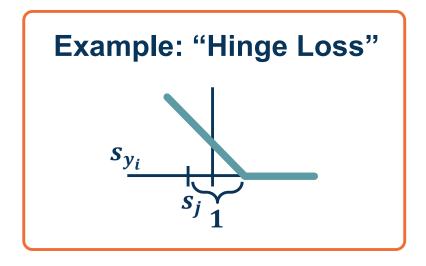
Given an example (x_i, y_i) where x_i is the image and where y_i is the (integer) label,



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

the SVM loss has the form:

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





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:

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

 $= \max(0, 5.1 - 3.2 + 1)$ $+ \max(0, -1.7 - 3.2 + 1)$

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

= 2.9 + 0

= 2.9

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







cat

car

frog

Losses:

3.2

5.1

-1.7

2.9

1.3

4.9

2.0

2.2

2.5

-3.1

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:

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

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

 $= \max(0, -2.6) + \max(0, -1.9)$

= 0 + 0

= 0

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







cat

car

frog

3.2

5.1

-1.7

Losses:

1.3

4.9

2.0

0.0

2.2

2.5

-3.1



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

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

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

No change for small values

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



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)
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Q: What is min/max of loss value?

[0,inf]

	w/	
Q	P	





cat	3.2	1.3	2.2
car	5.1	4.9	2.5

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

frog

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

Q: At initialization W is small so all s ≈ 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

-1.7 2.0

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

frog

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

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

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

No difference (add constant 1)







cat

3.2

1.3

2.2

car

5.1

4.9

2.5

frog

-1.7

2.0

-3.1

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 if we used mean instead of sum?

No difference Scaling by constant







cat

3.2

1.3

2.2

car

5.1

4.9

2.5

frog

-1.7

2.0

-3.1

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:

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

$$L = (2.9 + 0 + 12.9)/3$$

= **5.27**

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







- 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



- 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)

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

 $\min_{w} KL(p^*||\hat{p}) = \sum_{y} p^*(y) \log \frac{p^*(y)}{\hat{p}(y)}$ $= \sum_{y} p^*(y) \log(p^*(y)) - \sum_{y} p^*(y) \log(\hat{p}(y))$ $-H(p^*) \qquad \qquad H(p^*, \hat{p})$ (negative entropy, term goes away because not a function of model, W, parameters we are minimizing over)

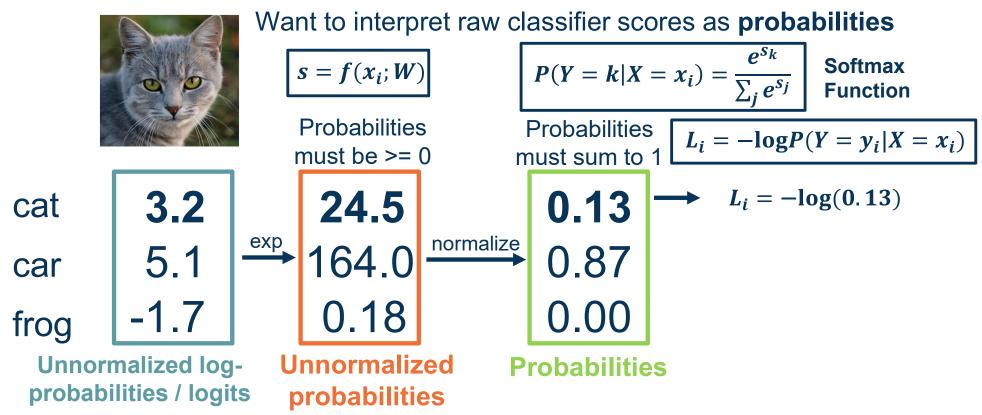
Ground Truth

Prediction

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



Softmax Classifier (Multinomial Logistic Regression)





Softmax Classifier (Multinomial Logistic Regression)



Want to interpret raw classifier scores as probabilities

$$s = f(x_i; W)$$

Probabilities must be >= 0

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

Probabilities must sum to 1 $L_i = -\log P(Y = y_i | X = x_i)$

$$L_i = -\log(0.13)$$

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

Infimum is 0, max is unbounded (inf)



Softmax Classifier (Multinomial Logistic Regression)



Want to interpret raw classifier scores as probabilities

$$s = f(x_i; W)$$

Probabilities must be >= 0

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

Probabilities must sum to 1 $L_i = -\log P(Y = y_i | X = x_i)$

$$L_i = -\log(0.13)$$

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

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



Often, we add a **regularization term** to the loss function

L1 Regularization
$$L_i = |y - Wx_i|^2 + |W|$$

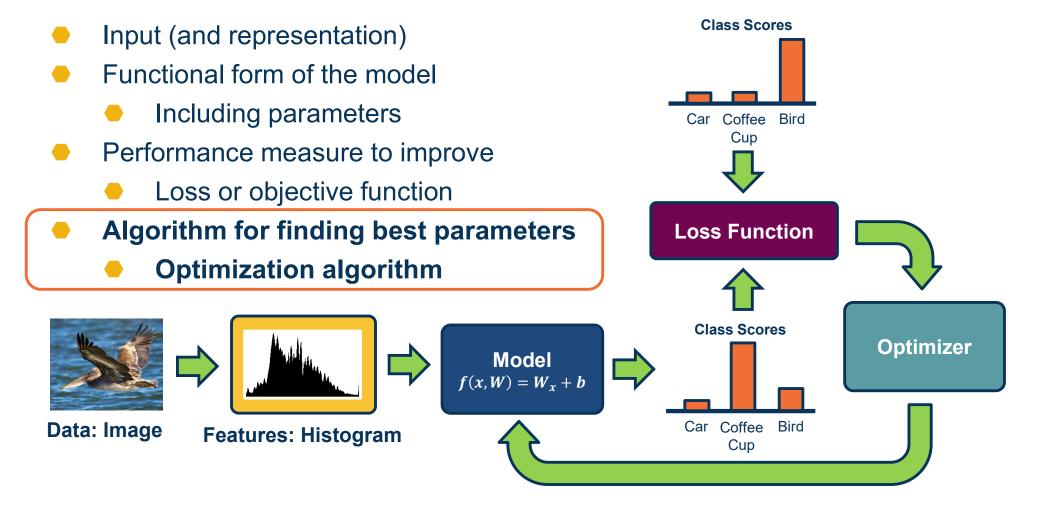
Example regularizations:

L1/L2 on weights (encourage small values)



Gradient Descent







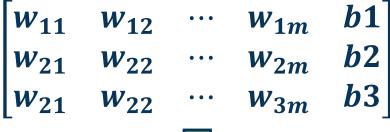
Given a model and loss function, finding the best set of weights is a **search problem**

 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





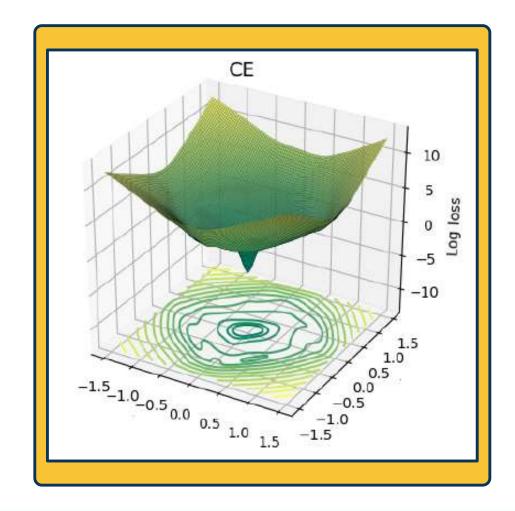
Loss



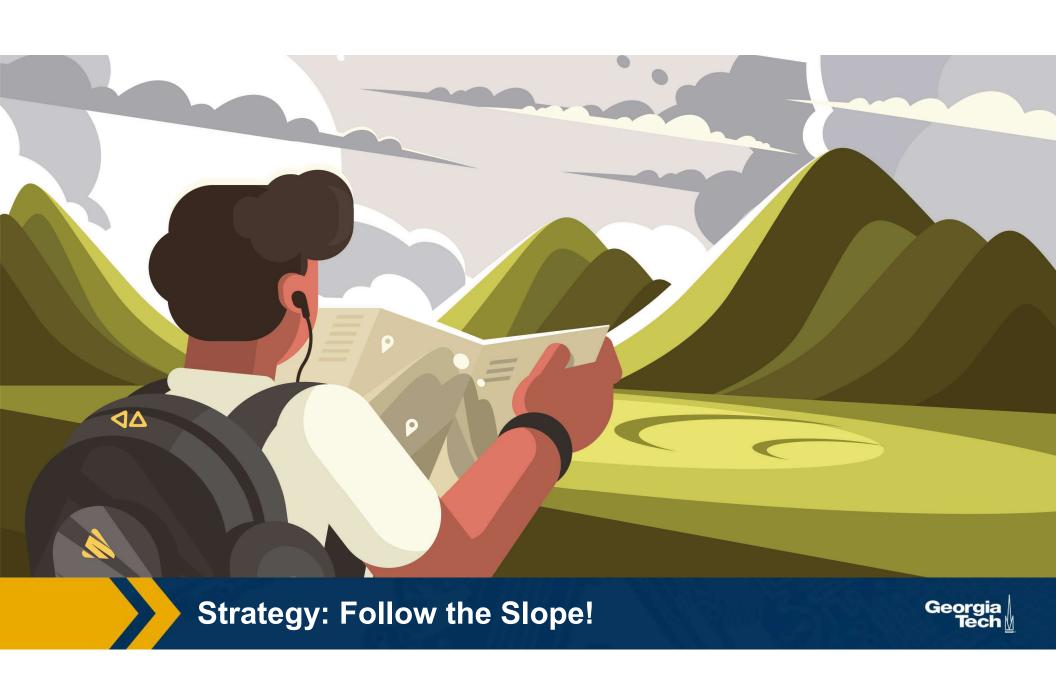
As weights change, the loss changes as well

 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

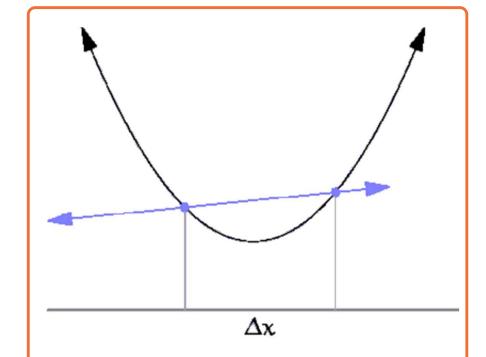


Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/ File:Tangent_animation.gif

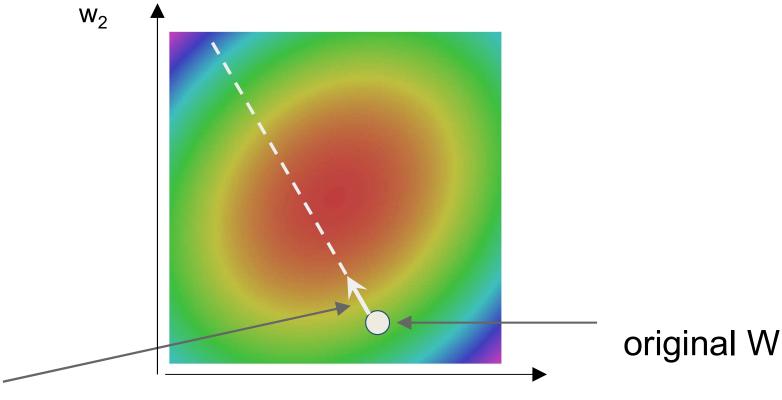


This idea can be turned into an algorithm (gradient descent)

- 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)



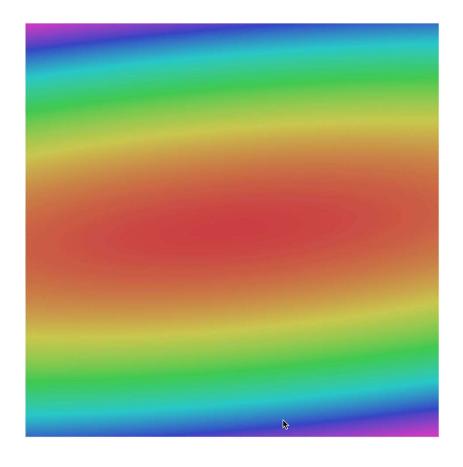
http://demonstrations.wolfram.com/VisualizingTheGradientVector/

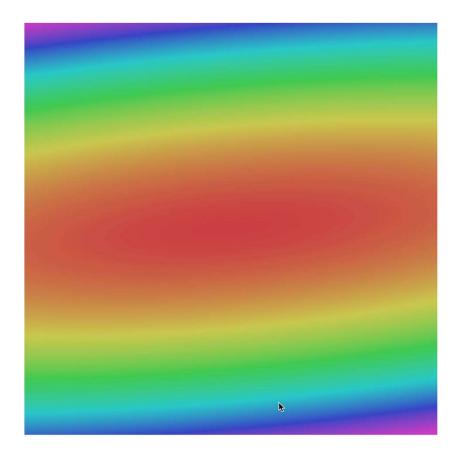


negative gradient direction

W







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

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

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

- 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

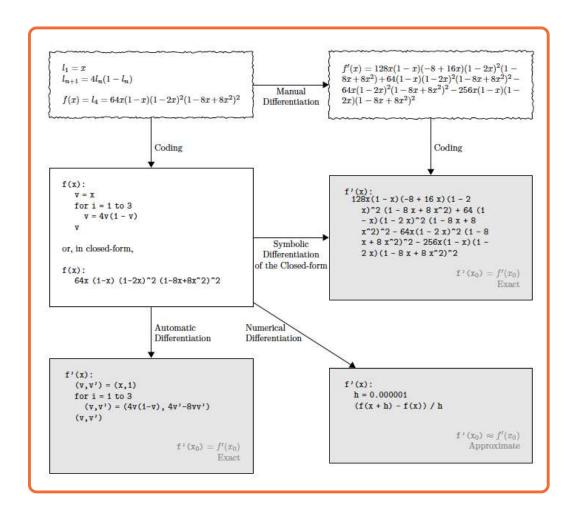
- For example, learning rate has to be appropriately reduced throughout training
- It will converge to a local minima
 - Small changes in weights would not decrease the loss
- It turns out that some of the local minima that it finds in practice (if trained well) are still pretty good!



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





current W:

[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...]

gradient dW:

W + h (first dim): current W: gradient dW: [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

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: [-2.5, ?, ?, ?, (1.25322 - 1.25347)/0.0001 = -2.5 $\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$?, ?,...]

W + h (second dim): current W: gradient dW: [0.34,[0.34, [-2.5, -1.11, -1.11 + 0.00010.78, 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 1.25353

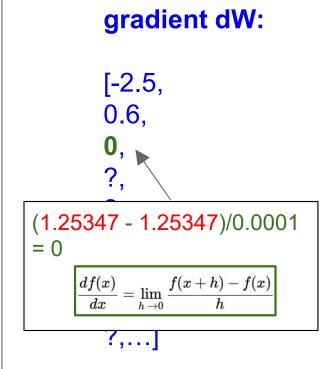
W + h (second dim): current W: [0.34, [0.34, -1.11, -1.11 + 0.00010.78, 0.78, 0.12, 0.12, 0.55, 0.55, 2.81, 2.81, = 0.6-3.1, -3.1, -1.5, -1.5, 0.33,...] 0.33,...] loss 1.25347 loss 1.25353

gradient dW:

[-2.5,
0.6,
?,
?,
(1.25353 - 1.25347)/0.0001
= 0.6
$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$
?,...]

W + h (third dim): current W: gradient dW: [0.34,[0.34, [-2.5,-1.11, -1.11, 0.6, 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

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



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:

Derivation of Update Rule

Function

Loss

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

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

Update Rule

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

For some functions, we can analytically derive the partial derivative

Example:

Function

Loss

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

(Assume w and 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

$$L = \sum_{k=1}^{N} (y_k - w^T x_k)^2$$

Gradient descent tells us we should update w as follows to minimize *L*:

$$w_j \leftarrow w_j - \eta \frac{\partial L}{\partial w_j}$$

So what's
$$\frac{\partial L}{\partial w_i}$$
?

$$\begin{aligned} \mathsf{L} &= \sum_{k=1}^{N} (y_k - w^T x_k)^2 & \frac{\partial L}{\partial w_j} = \sum_{k=1}^{N} \frac{\partial}{\partial w_j} (y_k - w^T x_k)^2 \\ &= \sum_{k=1}^{N} 2 \big(y_k - w^T x_k \big) \frac{\partial}{\partial w_j} (y_k - w^T x_k) \\ &= \sum_{k=1}^{N} 2 \big(y_k - w^T x_k \big) \frac{\partial}{\partial w_j} (y_k - w^T x_k) \\ &= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} w^T x_k \\ &= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{M} w_i x_{ki} \\ &= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{M} w_i x_{ki} \end{aligned}$$

If we add a non-linearity (sigmoid), derivation is more complex

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

First, one can derive that: $\sigma'^{(x)} = \sigma(x)(1 - \sigma(x))$

$$f(x) = \sigma\left(\sum_{k} w_{k} x_{k}\right)$$

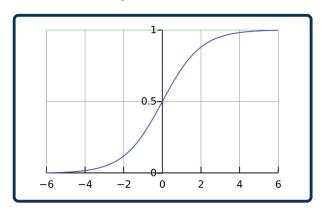
$$L = \sum_{i} \left(y_{i} - \sigma \left(\sum_{k} w_{k} x_{ik} \right) \right)^{2}$$

$$\frac{\partial L}{\partial w_j} = \sum_{i} 2 \left(y_i - \sigma \left(\sum_{k} w_k x_{ik} \right) \right) \left(-\frac{\partial}{\partial w_j} \sigma \left(\sum_{k} w_k x_{ik} \right) \right)$$

$$= \sum_{i} -2 \left(y_i - \sigma \left(\sum_{k} w_k x_{ik} \right) \right) \sigma' \left(\sum_{k} w_k x_{ik} \right) \frac{\partial}{\partial w_j} \sum_{k} w_k x_{ik}$$

$$= \sum_{i} -2 \delta_i \sigma(\mathbf{d}_i) (1 - \sigma(\mathbf{d}_i)) x_{ij}$$

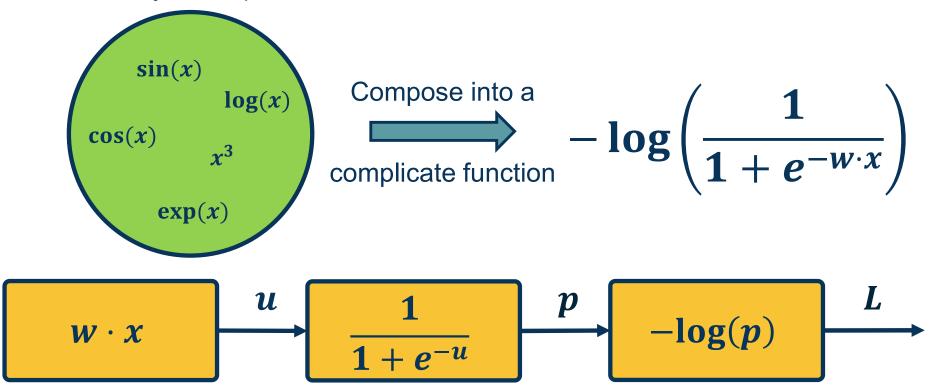
where
$$\delta_i = y_i - f(x_i)$$
 $d_i = \sum w_k x_{ik}$



The sigmoid perception update rule:

$$w_j \leftarrow w_j + 2\eta \sum_{k=1}^N \delta_i \sigma_i (1-\sigma_i) x_{ij}$$
 where $\sigma_i = \sigma \Biggl(\sum_{j=1}^m w_j x_{ij}\Biggr)$ $\delta_i = y_i - \sigma_i$

Given a library of simple functions



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

