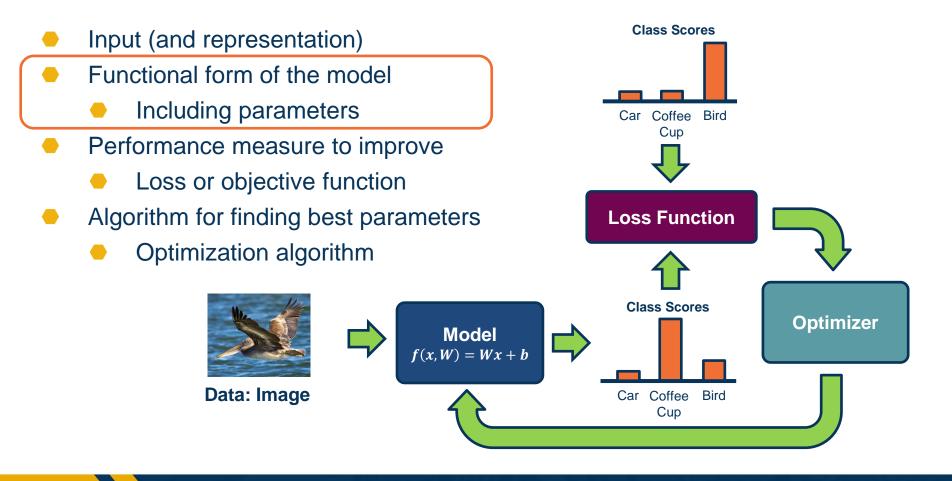
Topics:

- Linear Classification, Loss functions
- Gradient Descent

CS 4644-DL / 7643-A ZSOLT KIRA

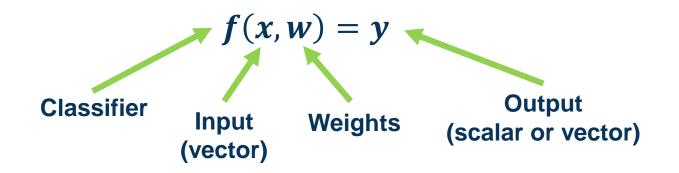
• Assignment 1 out!

- Due Feb. 2nd 11:59pm (grace period Feb 4th).
- Start early, start early, start early!
- HW1 Tutorial, Matrix Calculus tutorial OH: TBA
- **Piazza:** Should be sync'd with Canvas now (Code: DLSPR2024)
 - **NOTE:** There is an OMSCS section with a Ed. Make sure you are in the right one
- Tentative Office hours schedule: <u>https://piazza.com/class/lcl94yjxkbb59e/post/53</u>
 - Calendar on webpage: <u>https://faculty.cc.gatech.edu/~zk15/teaching/AY2024_cs7643_spring/ind</u> ex.html



Components of a Parametric Model

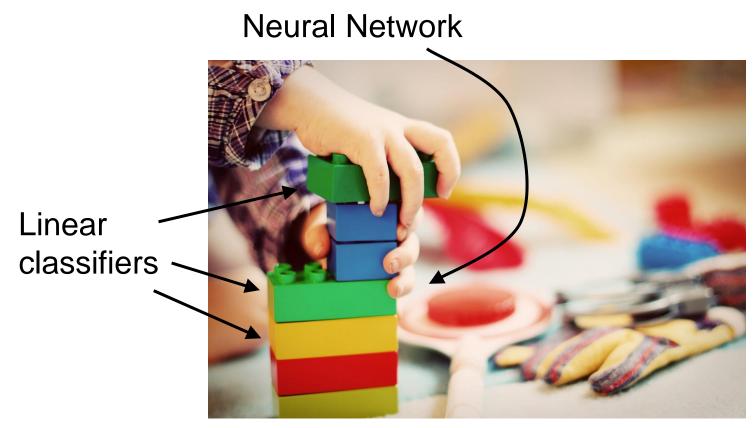




- Input: Continuous number or vector
- Output: A continuous number
 - For classification typically a **score**
 - For regression what we want to regress to (house prices, crime rate, etc.)
- w is a vector and weights to optimize to fit target function

Model: Discriminative Parameterized Function





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

Deep Learning as Legos



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

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

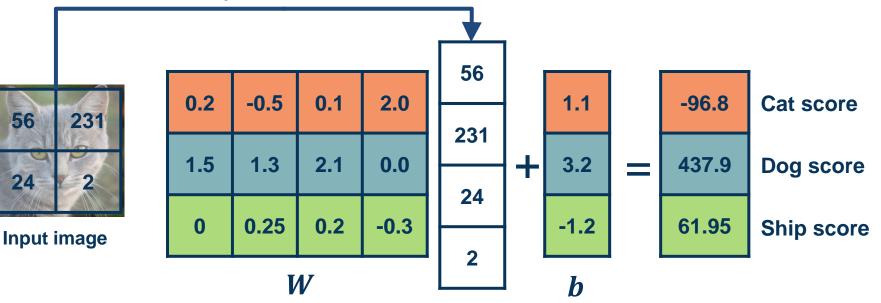
W

X





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



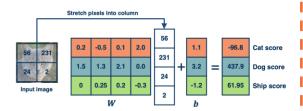
Stretch pixels into column







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



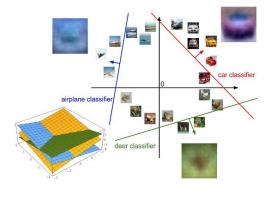
Visual Viewpoint

One template per class



Geometric Viewpoint

Hyperplanes cutting up space



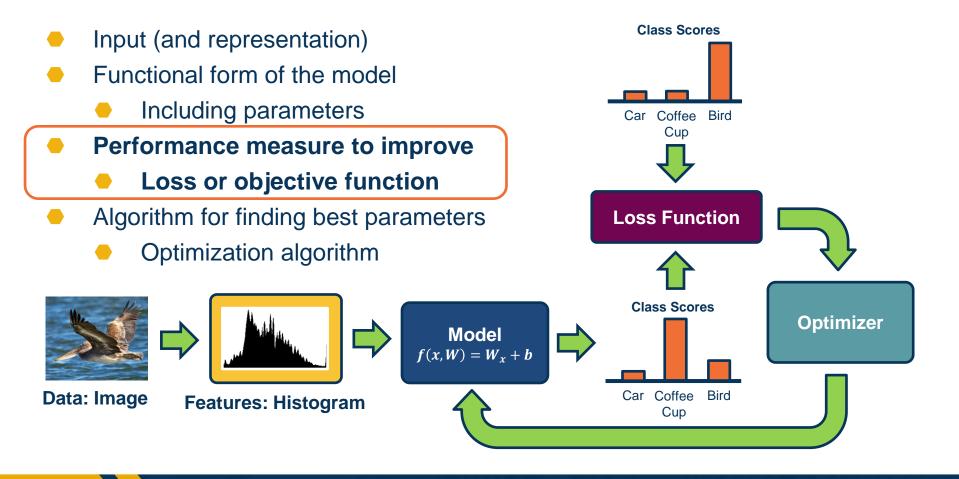
Adapted from slides by Fei-Fei Li, Justin Johnson, Serena Yeung, from CS 231n

Linear Classifier: Three Viewpoints



Performance Measure for a Classifier

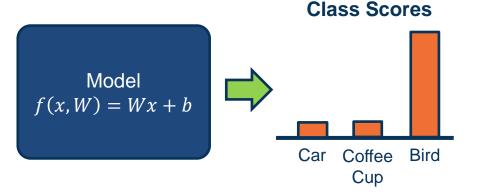




Components of a Parametric Model

Georgia Tech

- 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

Converting Scores to Probabilities



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:

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

Performance Measure



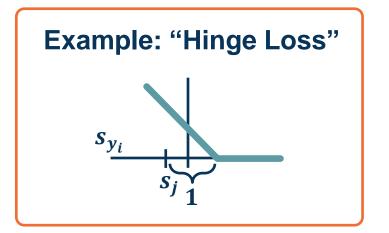
Given an example (x_i, y_i) where x_i is the image and where y_i is the (integer) label,



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

the SVM loss has the form:

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



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

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: $s = f(x_i, W)$

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

the SVM loss has the form:

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

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

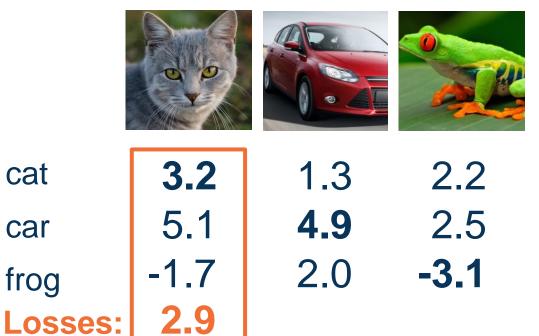
 $= \max(0, 2.9) + \max(0, -3.9)$

 $L_i =$

= 2.9 + 0

= 2.9

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







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: $s = f(x_i, W)$

 $\max_{i \in y_i} \max(0, s_j - s_{y_i} + 1)$

the SVM loss has the form:

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

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

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

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



= 0 + 0= 0

 $L_i =$





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

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:



3.2	1.3	2.2
5.1	4.9	2.5
-1.7	2.0	-3.1

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



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





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

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
frog	-1.7	2.0	-3.1





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

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





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

Q: What if we used mean instead of sum?

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



	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





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: $s = f(x_i, W)$

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



the SVM loss has the form:	cat	3.2	1.3	2.2
$L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$	car	5.1	4.9	2.5
	frog	-1.7	2.0	-3.1
L = (2.9 + 0 + 12.9)/3 = 5.27	Losses:	2.9	0	12.9





- 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)

w

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

Ground Truth



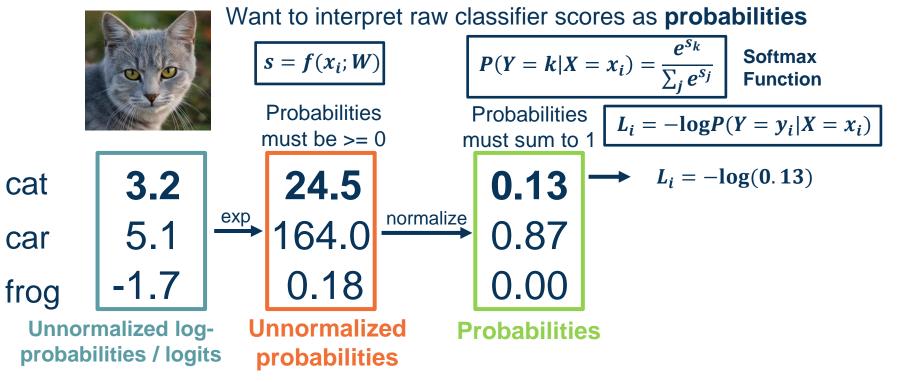
$$\begin{split} \min_{w} KL(p^*||\hat{p}) &= \sum_{y} p^*(y) \log \frac{p^*(y)}{\hat{p}(y)} \\ &= \sum_{y} p^*(y) \log(p^*(y)) - \sum_{y} p^*(y) \log(\hat{p}(y)) \\ & -H(p^*) & H(p^*, \hat{p}) \\ \text{(negative entropy, term goes away)} \\ \text{because not a function of model, } W, \\ \text{parameters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

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)







Softmax Classifier (Multinomial Logistic Regression)



Want to interpret raw classifier scores as probabilities

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

Probabilities must be $\geq = 0$

$$P(Y = k | X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$
Softmax
Function
Probabilities
The sum to 1 $L_i = -\log P(Y = y_i | X = x_i)$

must sum to 1

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

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 $\geq = 0$

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

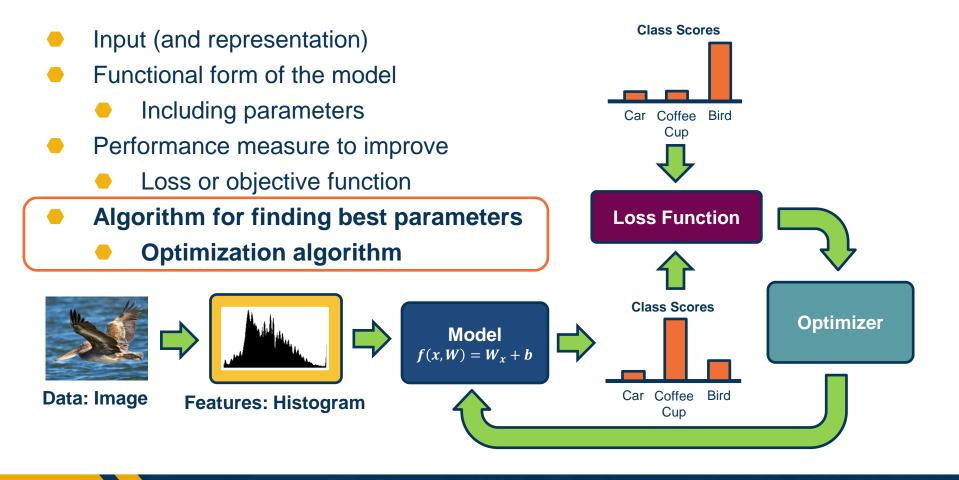
L1/L2 on weights (encourage small values)





Gradient Descent





Components of a Parametric Model

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

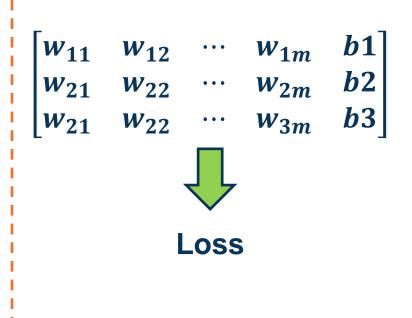
 Find the best combination of weights that minimizes our loss function

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

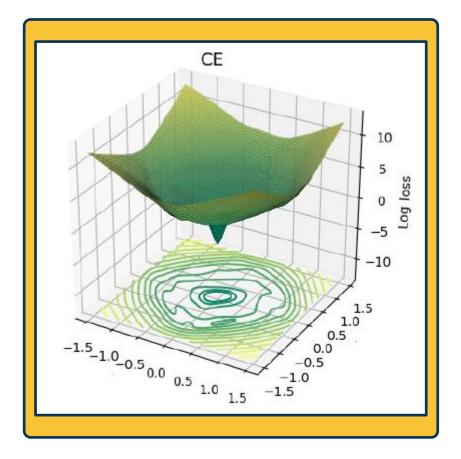




As weights change, the loss changes as well

 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









0

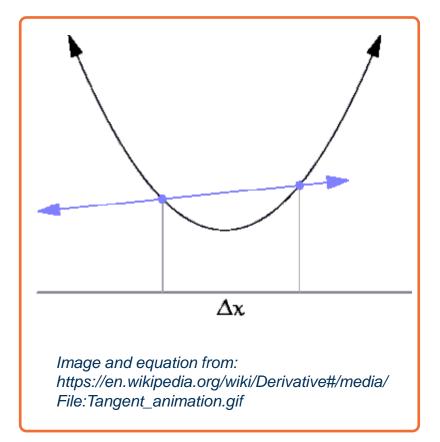
dΔ



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

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

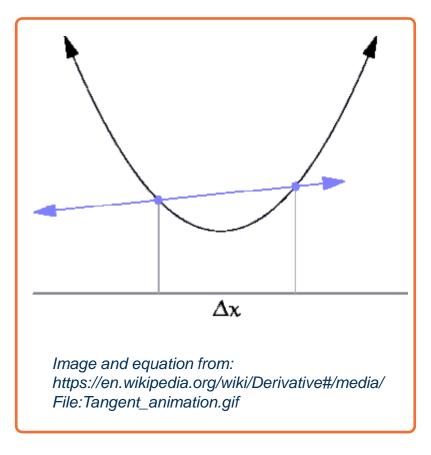
- Steepest descent direction is the negative gradient
- Intuitively: Measures how the function changes as the argument a changes by a small step size
 - As step size goes to zero
- In Machine Learning: Want to know how the loss function changes as weights are varied
 - Can consider each parameter separately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







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





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

- 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: $w_i = w_i \frac{\partial L}{\partial w_i}$

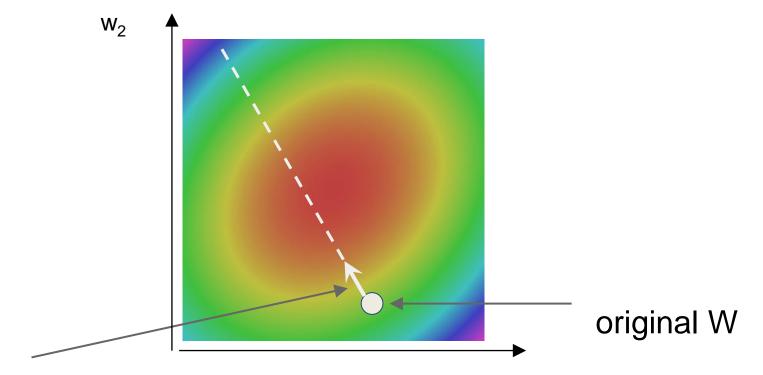
Add learning rate to prevent too big of a step: $w_i = w_i - \alpha \frac{\partial L}{\partial w_i}$

5. Repeat (from Step 3)





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

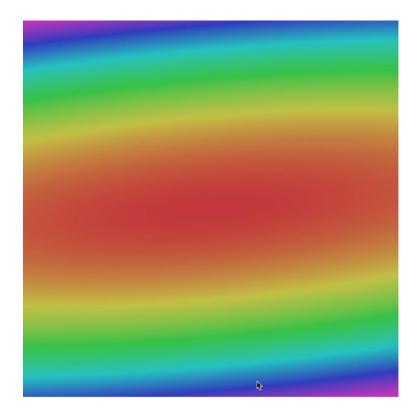


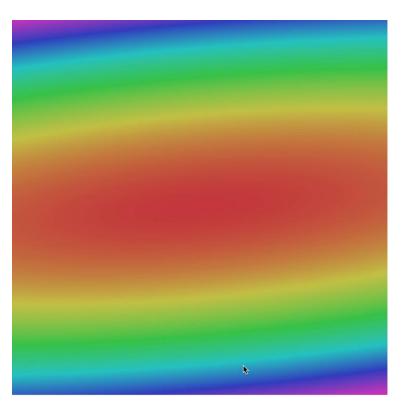
 W_1

GA

negative gradient direction







 W_1





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!

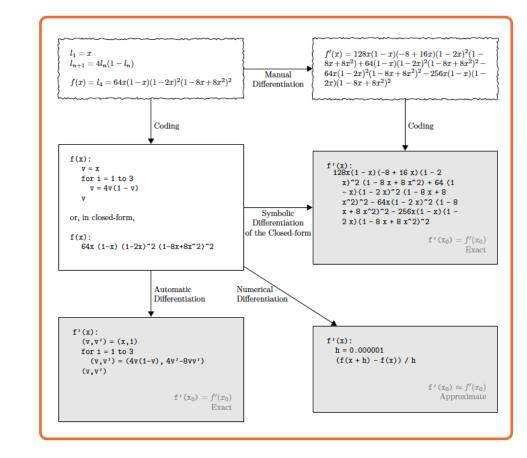




We know how to compute the **model output and loss** function

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

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



Computing Gradients



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

V:

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:

[?,

?,

?,

?,

?,

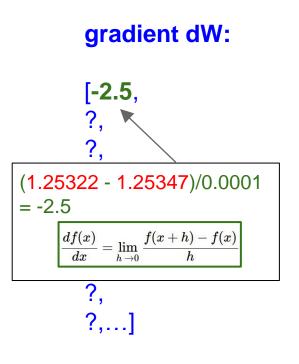
?,

?,

?,

?,...]

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



current W:	W + h (second dim):	gradi
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11 + 0.0001 ,	?,
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,]	?,
Ioss 1.25347	Joss 1.25353	?,]

gradient dW:

current W:	W + h (second dim):	gradient dW:
[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, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6

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,

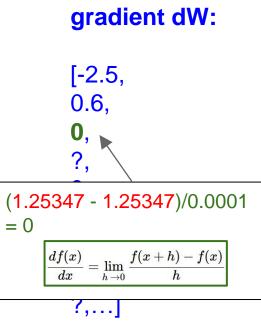
0.6,

?,

?,

?, ?, ?, ?,...]

current W:	W + h (third dim):	gradien
[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,]	[0.34, -1.11, 0.78 + 0.0001 , 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,]	[-2.5, 0.6, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,



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 **Derivation of Update Rule Example:** Loss **Function** $f(w, x_i) = w^T x_i \qquad (y_i - w^T x_i)^2$ (Assume w and \mathbf{x}_i are column vectors, so same as $w \cdot x_i$) **Update Rule** $w_j \leftarrow w_j + 2\alpha \sum_{k=1}^N \delta_k x_{kj}$





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 $w \cdot x_i$)

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

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

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

$$L = \sum_{k=1}^{N} (y_k - w^T x_k)^2 \qquad \frac{\partial L}{\partial w_j} = \sum_{k=1}^{N} \frac{\partial}{\partial w_j} (y_k - w^T x_k)^2$$
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 $\frac{\partial L}{\partial w_j}$?

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} w^T x_k$$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{m} w_i x_{ki}$$

$$= -2 \sum_{k=1}^{N} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{m} w_i x_{ki}$$

Manual Differentiation



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

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

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

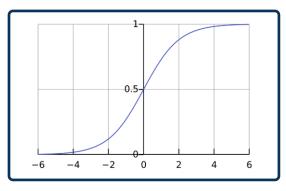
$$f(\mathbf{x}) = \sigma\left(\sum_{k} w_{k} x_{k}\right)$$

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

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

$$= \sum_{i} -2\left(y_{i} - \sigma\left(\sum_{k} w_{k} x_{ik}\right)\right) \sigma'\left(\sum_{k} w_{k} x_{ik}\right) \frac{\partial}{\partial w_{j}} \sum_{k} w_{k} x_{ik}$$

$$= \sum_{i} -2\delta_{i}\sigma(\mathbf{d}_{i})(1 - \sigma(\mathbf{d}_{i}))x_{ij}$$
where $\delta_{i} = y_{i} - \mathbf{f}(x_{i})$ $d_{i} = \sum_{i} w_{k} x_{ik}$



The sigmoid perception update rule:

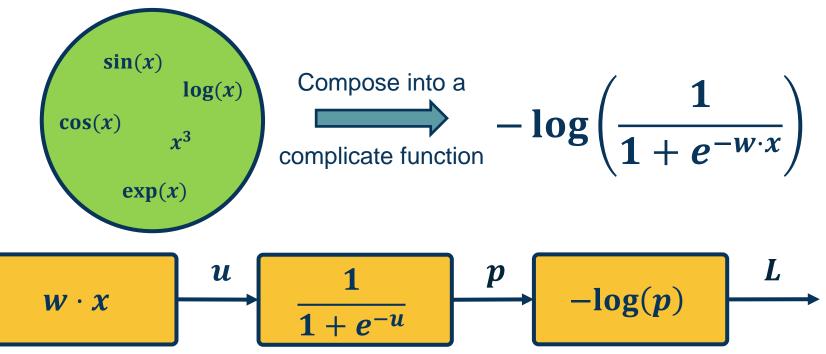
$$w_{j} \leftarrow w_{j} + 2\alpha \sum_{k=1}^{N} \delta_{i} \sigma_{i} (1 - \sigma_{i}) x_{ij}$$

where $\sigma_{i} = \sigma \left(\sum_{j=1}^{m} w_{j} x_{ij} \right)$
 $\delta_{i} = y_{i} - \sigma_{i}$

Adding a Non-Linear Function



Given a library of simple functions



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



