Topics:

- Linear Classification, Loss functions
- Gradient Descent

CS 4803-DL / 7643-A
ZSOLT KIRA

- **Assignment 1 out today!**
  - Start early, start early, start early!

- **Piazza:** Enroll now! https://piazza.com/class/kjsselshfiz18c (Code: DL2021)
  - **NOTE:** There is an OMSCS section with a DIFFERENT piazza. Make sure you are in the right one

- **Office hours** start this week

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**

Parametric – Linear Classifier

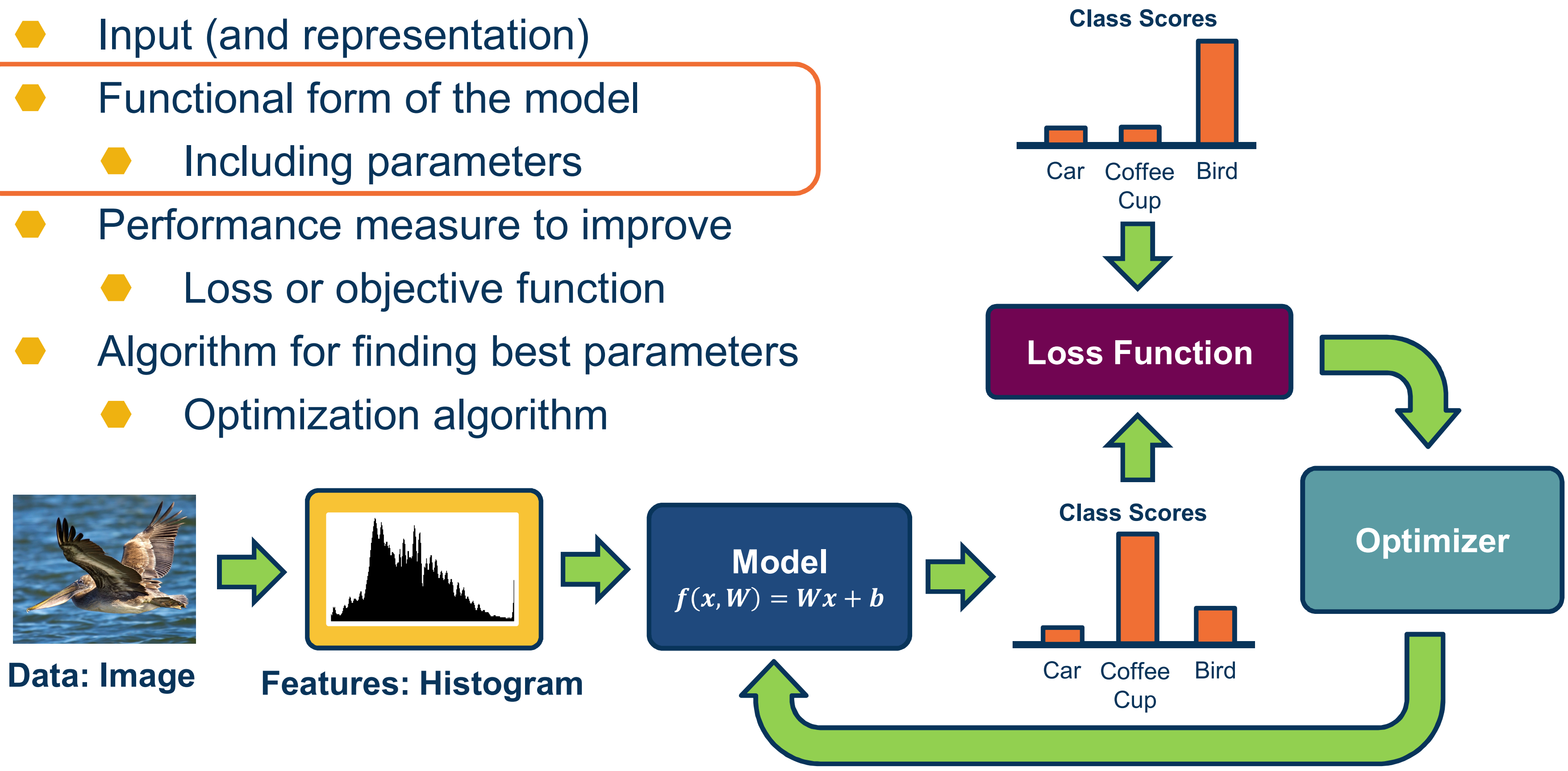
$$f(x, W) = Wx + b$$

Procedure:

Calculate score per class for example

Return label of maximum score (argmax)

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



Components of a Parametric Model

$$f(x, w) = y$$

Classifier · **Input (vector)** · **Weights** · **Output (scalar or vector)**

- **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

Neural Network

Linear
classifiers

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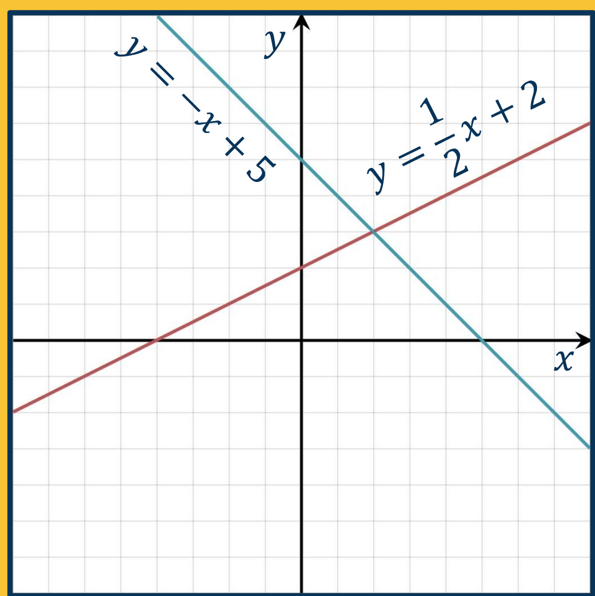
Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Deep Learning as Legos

Georgia Tech

What is the **simplest function** you can think of?

$$y = mx + b$$



Our model is:

$$f(x, w) = w \cdot x + b$$

Classifier Result

Weights

Input

Bias (scalar)

(Note if w and $\mathbf{x}$ are column vectors we often show this as $w^T x$)

Image adapted from: https://en.wikipedia.org/wiki/Linear_equation#/media/File:Linear_Function_Graph.svg

Simple Function

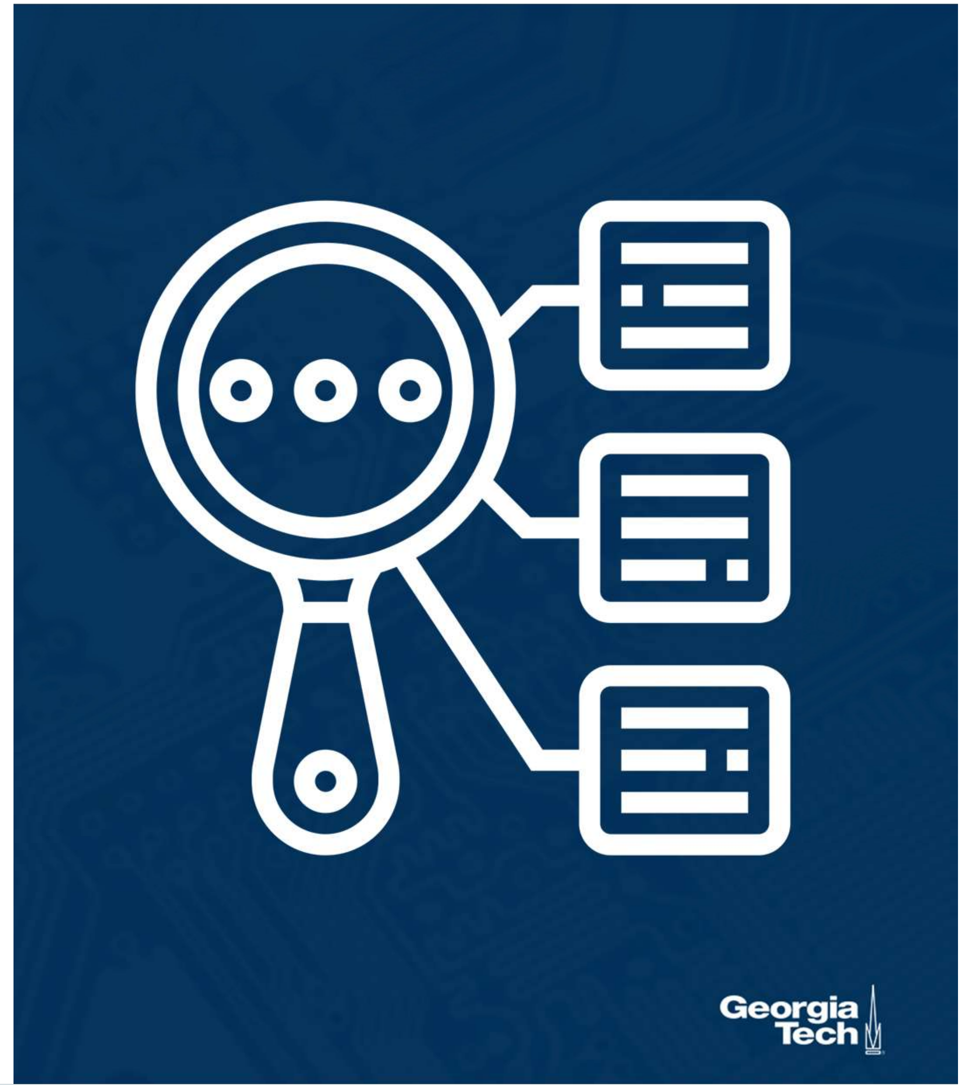
Linear Classification and Regression

Simple linear classifier:

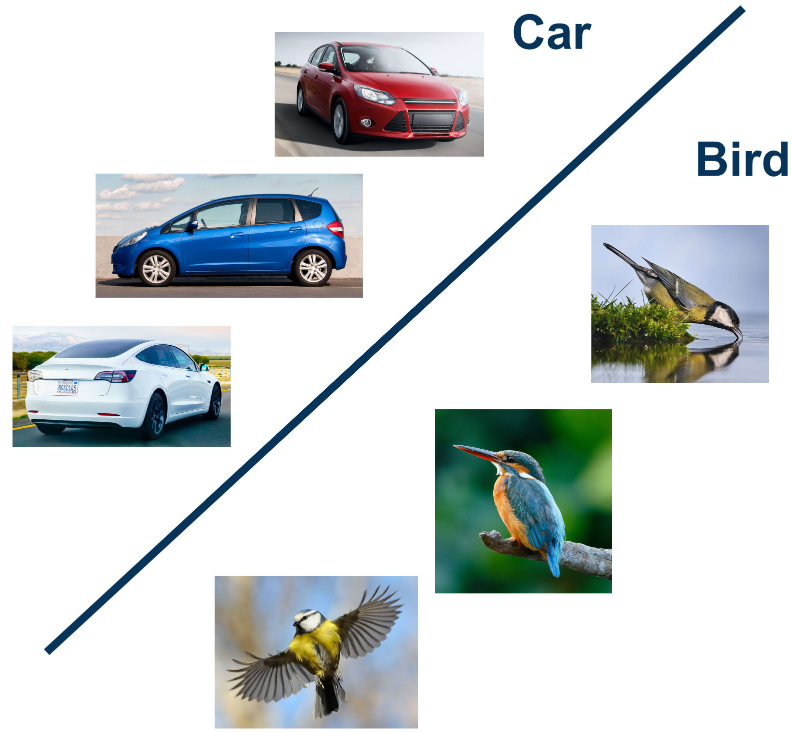
- Calculate score:
  $f(x, w) = w \cdot x + b$
- Binary classification rule (w is a vector):

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

- For multi-class classifier take class with highest (max) score
  $f(x, W) = Wx + b$



- **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



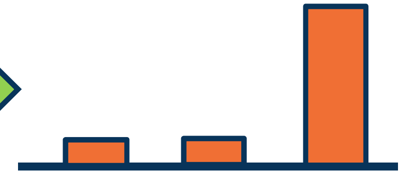
Input Dimensionality

Data: Image

Model

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

Class Scores



$$x = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nn} \end{bmatrix}$$

Flatten

$$x = \begin{bmatrix} x_{11} \\ x_{12} \\ \vdots \\ x_{21} \\ x_{22} \\ \vdots \\ x_{n1} \\ \vdots \\ x_{nn} \end{bmatrix}$$

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 →
Classifier for class 2 →
Classifier for class 3 →

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

$$\boldsymbol{W} \qquad \boldsymbol{x} \qquad \boldsymbol{b}$$

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

Weights

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

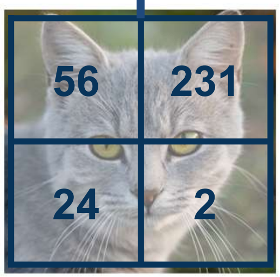
- We can move the bias term into the weight matrix, and a "1" at the end of the input
- Results in **one matrix-vector multiplication**!

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

Weights

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

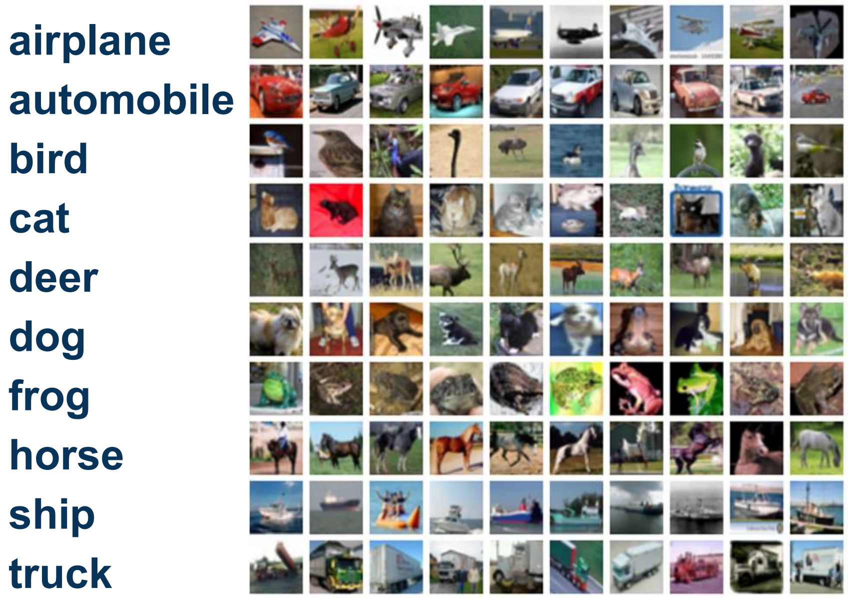
Stretch pixels into column



Input image

$$\underbrace{\begin{bmatrix}0.2 & -0.5 & 0.1 & 2.0\\ 1.5 & 1.3 & 2.1 & 0.0\\ 0 & 0.25 & 0.2 & -0.3\end{bmatrix}}_{W}\begin{bmatrix}56\\ 231\\ 24\\ 2\end{bmatrix}+\underbrace{\begin{bmatrix}1.1\\ 3.2\\ -1.2\end{bmatrix}}_{b}=\begin{bmatrix}-96.8\\ 437.9\\ 61.95\end{bmatrix}\begin{matrix}\text{Cat score}\\ \text{Dog score}\\ \text{Ship score}\end{matrix}$$

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

Interpreting a Linear Classifier

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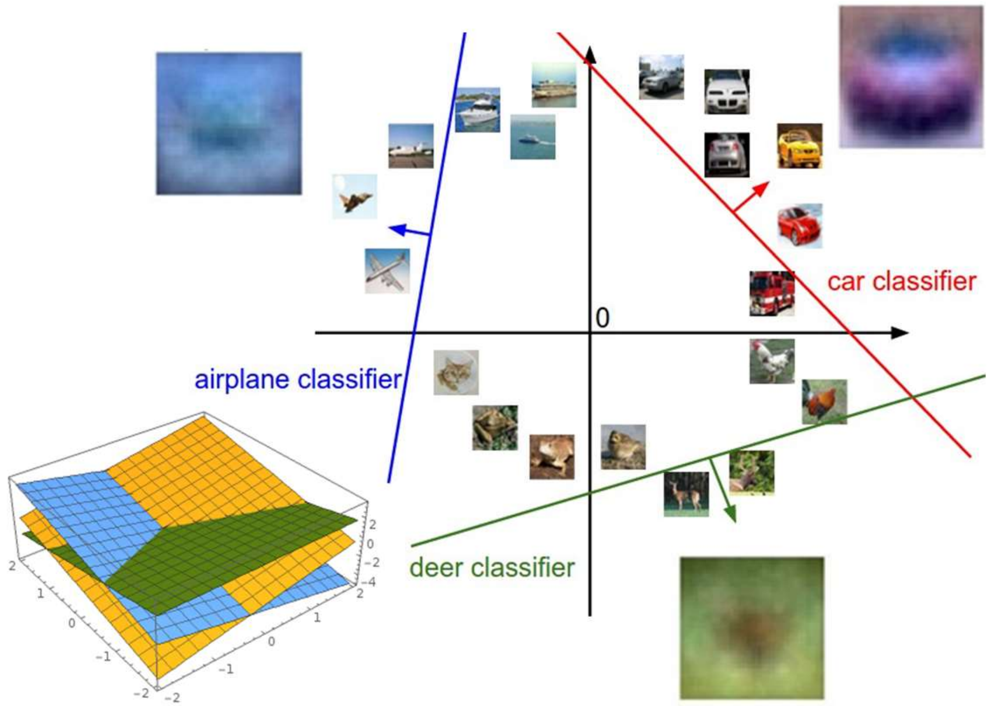
Geometric Viewpoint



Plot created using Wolfram Cloud

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

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

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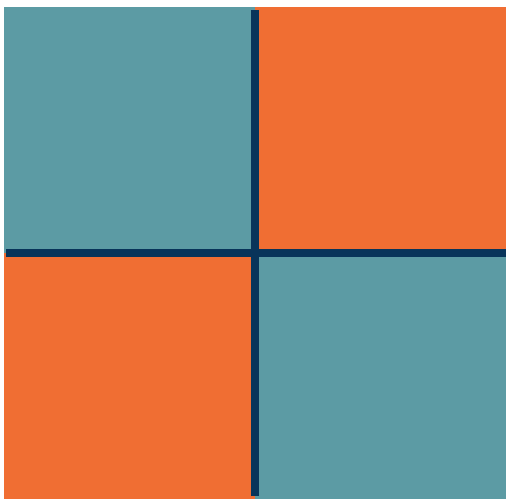
Hard Cases for a Linear Classifier

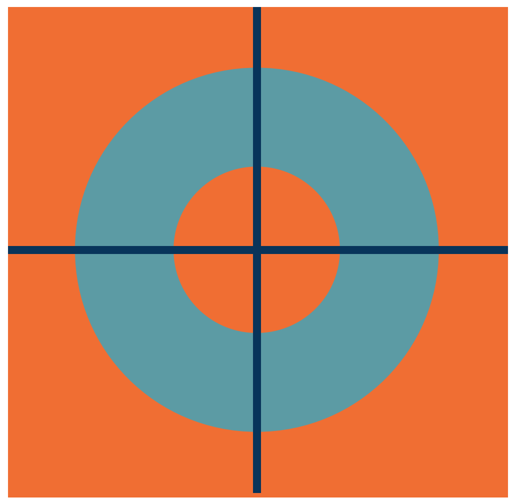
Class 1:
number of pixels > 0 odd

Class 2:
number of pixels > 0 even



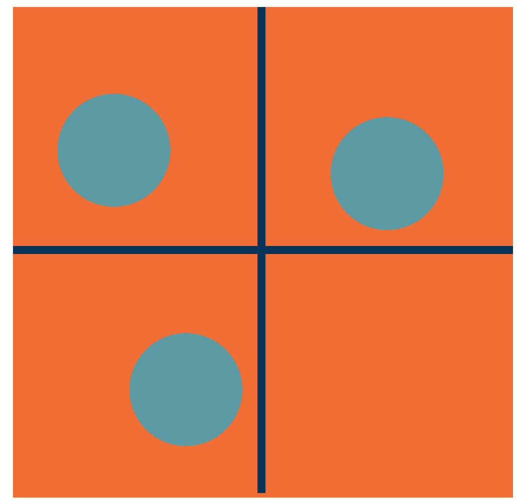
Class 1:
1 < = L2 norm < = 2

Class 2:
Everything else



Class 1:
Three modes

Class 2:
Everything else



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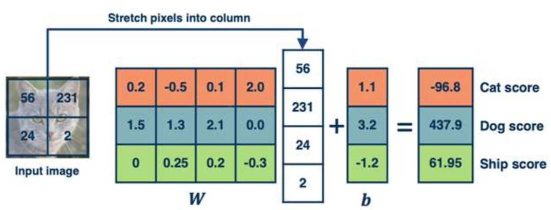
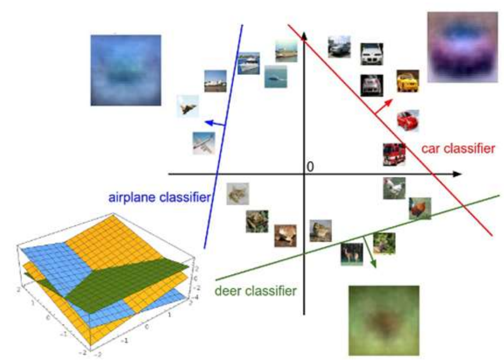
Linear Classifier: Three Viewpoints

Algebraic Viewpoint	Visual Viewpoint	Geometric Viewpoint
$f(x, W) = Wx$	One template per class	Hyperplanes cutting up space





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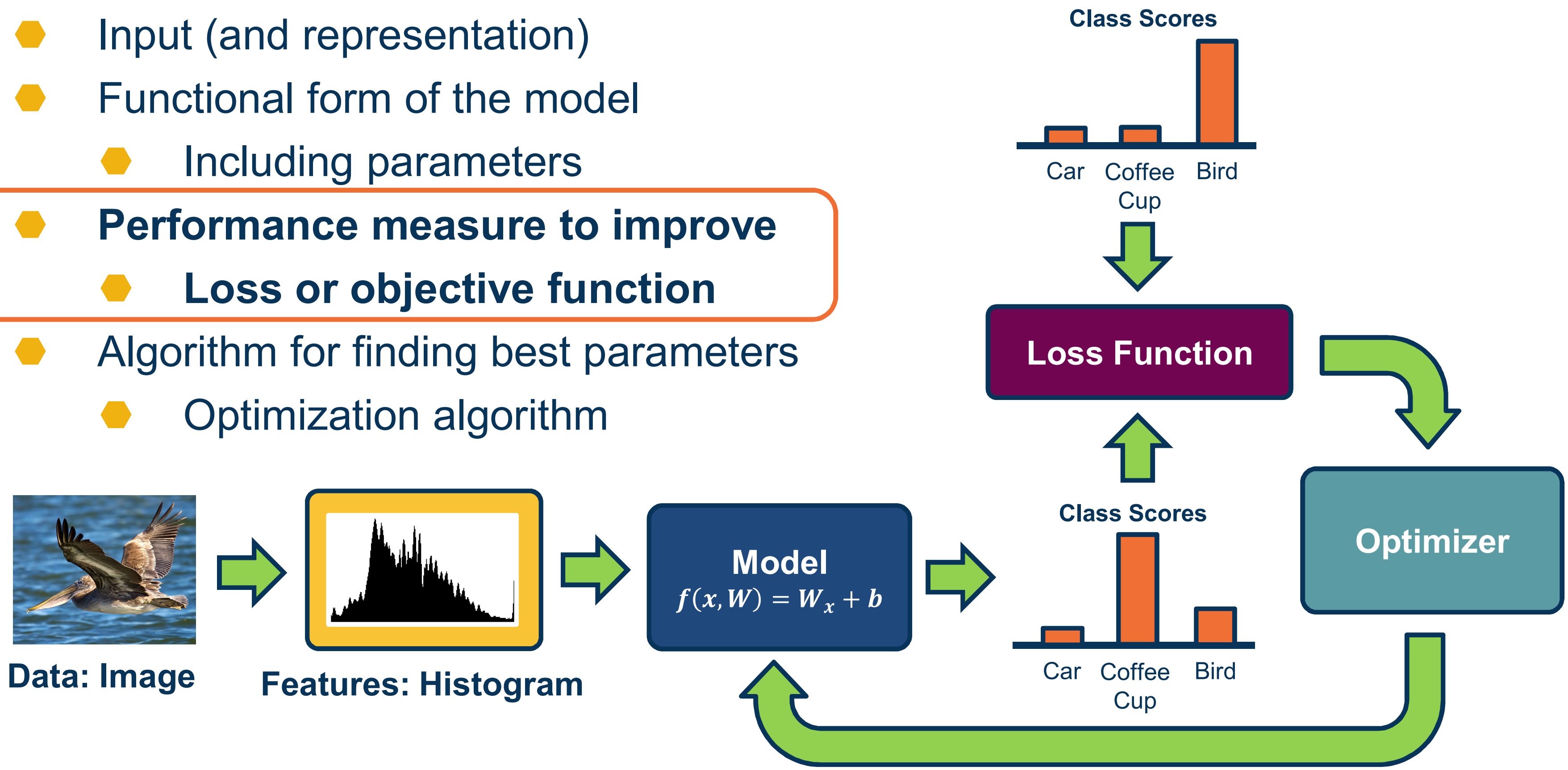
Performance Measure for a Classifier

- Input (and representation)
- Functional form of the model
  - Including parameters
- **Performance measure to improve**
  - **Loss or objective function**
- Algorithm for finding best parameters
  - Optimization algorithm

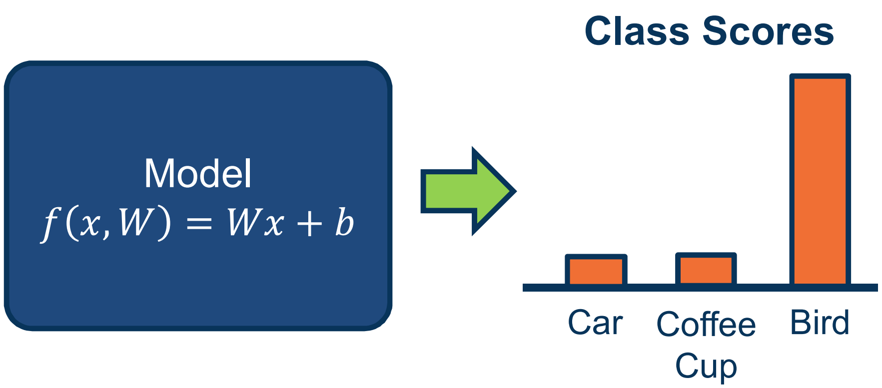


Components of a Parametric Model

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

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

  - 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

Performance Measure

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:

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

Where $\boldsymbol{x_i}$ is image and

$\boldsymbol{y_i}$ is (integer) label

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

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

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Multiclass SVM loss:

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

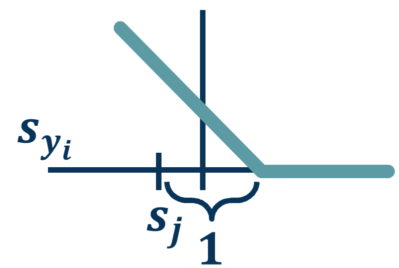
and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \begin{cases} 0 & \text{if } s_{y_i} \geq s_j + 1 \\ s_j - s_{y_i} + 1 & \text{otherwise} \end{cases}$$

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

Example: "Hinge Loss"



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Performance Measure for Scores

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Multiclass SVM loss:

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, 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	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	**2.9**		

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

Multiclass SVM loss:

Given an example $(\boldsymbol{x_i}, \boldsymbol{y_i})$ where $\boldsymbol{x_i}$ is the image and where $\boldsymbol{y_i}$ is the (integer) label,

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

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 $\boldsymbol{W}$ the scores $\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{W}) = \boldsymbol{W}\boldsymbol{x}$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
	Losses:	**0.0**	

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SVM Loss Example

Multiclass SVM loss:

Given an example $(\boldsymbol{x_i}, \boldsymbol{y_i})$
where $\boldsymbol{x_i}$ is the image and
where $\boldsymbol{y_i}$ is the (integer) label,

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

the SVM loss has the form:

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

L = (2.9 + 0 + 12.9)/3
= **5.27**

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



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

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SVM Loss Example

Multiclass SVM loss:

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

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:

			
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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Multiclass SVM loss:

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

Q: What is min/max of loss value?

[0,inf]

Suppose: 3 training examples, 3 classes.
With some $\boldsymbol{W}$ the scores $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{W})=\boldsymbol{W}\boldsymbol{x}$ 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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SVM Loss Example

SVM Loss Example

Multiclass SVM loss:

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

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

C-1

Suppose: 3 training examples, 3 classes.
With some $\boldsymbol{W}$ the scores $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{W})=\boldsymbol{W}\boldsymbol{x}$ 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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Multiclass SVM loss:

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

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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SVM Loss Example

Georgia Tech

Multiclass SVM loss:

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

Q: What if we used mean instead of sum?

No difference
Scaling by constant

Suppose: 3 training examples, 3 classes.
With some $\boldsymbol{W}$ the scores $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{W})=\boldsymbol{W}\boldsymbol{x}$ 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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SVM Loss Example

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

$$L = \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1)$$

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

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

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

Performance Measure for Probabilities

Georgia Tech

- If we use the softmax function to convert scores to probabilities, the right loss function to use is **cross-entropy**

Performance Measure for Probabilities

Georgia Tech

Softmax Classifier (Multinomial Logistic Regression)

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

$s = f(x_i; W)$

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

Probabilities must be >= 0

Probabilities must sum to 1

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

	Unnormalized log-probabilities / logits	exp →	Unnormalized probabilities	normalize →	Probabilities	
cat	**3.2**		**24.5**		**0.13**	→ $L_i = -\log(0.13)$
car	5.1		164.0		0.87	
frog	-1.7		0.18		0.00	

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

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)

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

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) ≈ 2

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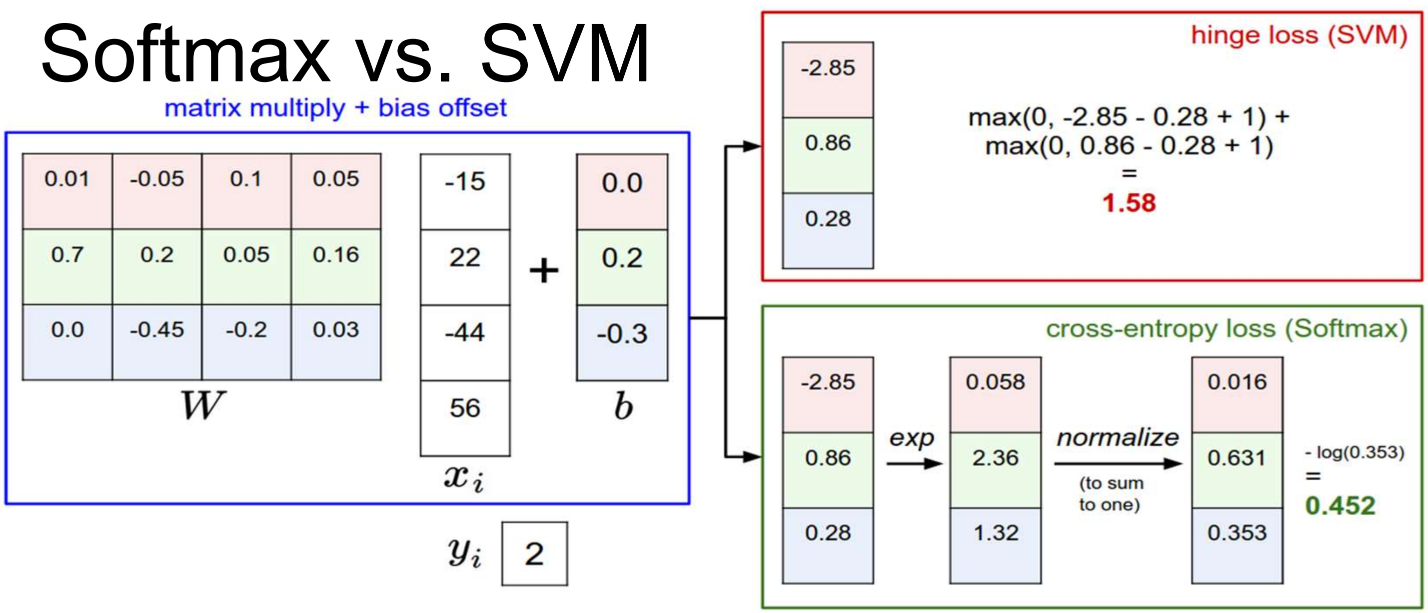

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Cross-Entropy Loss Example

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

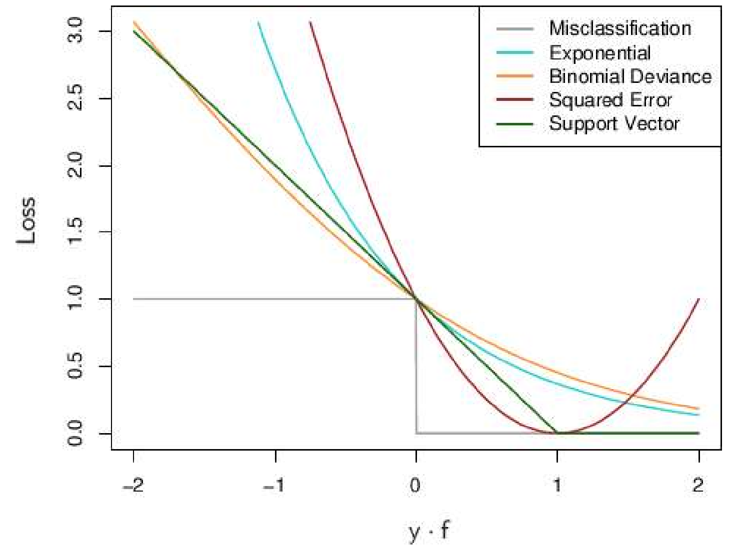
- **Example:** House price prediction

$$L_i = |y - Wx_i|$$ **L1**

$$L_i = |y - Wx_i|^2$$ **L2**

- For probabilities

$$L_i = |y - Wx_i| = \frac{e^{s_k}}{\sum_j e^{s_j}}$$ **Logistic**



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

Regression Example

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

L1 Regularization

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

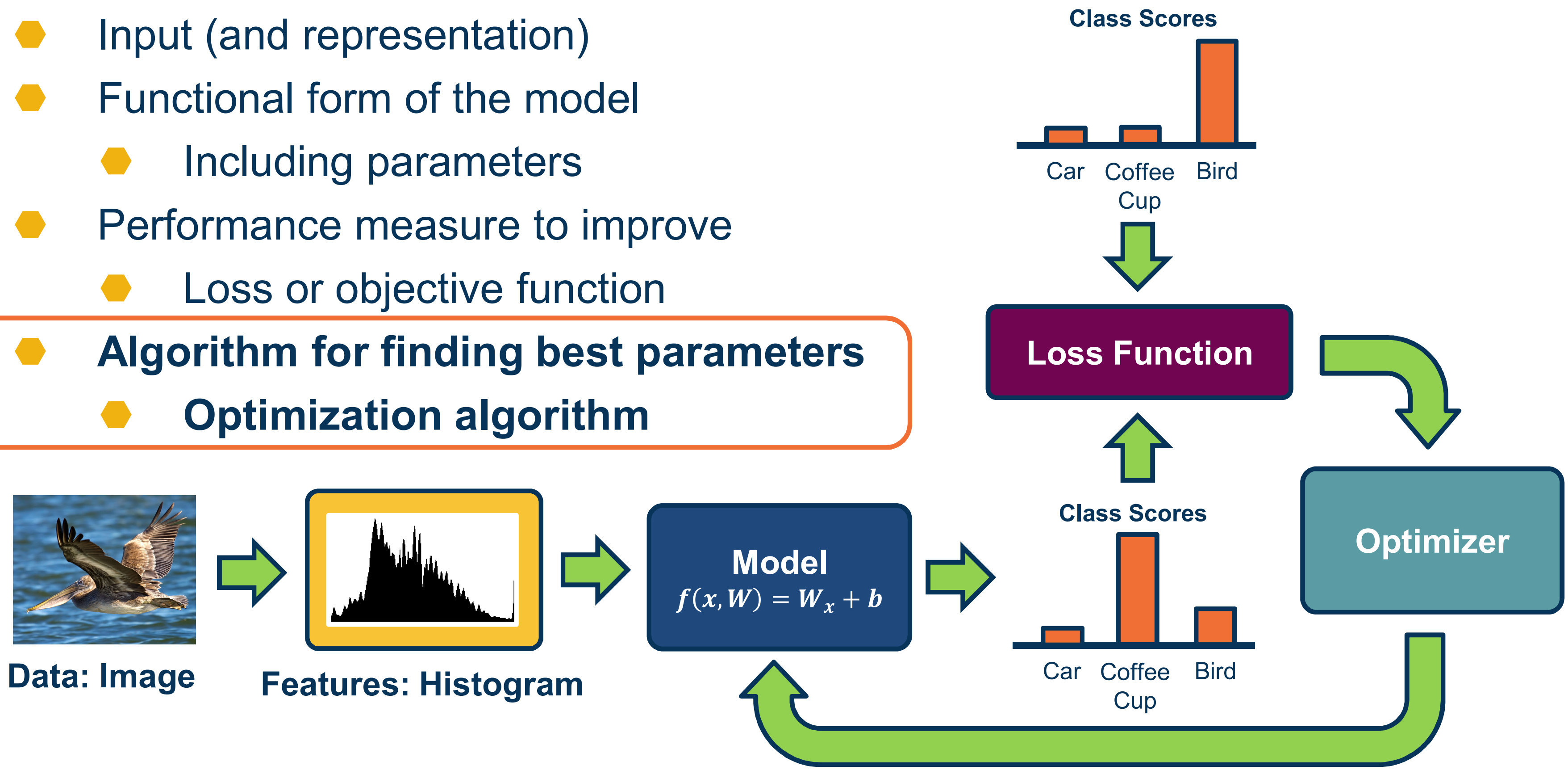
Example regularizations:

- L1/L2 on weights (encourage small values)

Gradient Descent

Components of a Parametric Model

- Input (and representation)
- Functional form of the model
  - Including parameters
- Performance measure to improve
  - Loss or objective function
- **Algorithm for finding best parameters**
  - **Optimization algorithm**



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

$$\begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} & b1 \\ w_{21} & w_{22} & \cdots & w_{2m} & b2 \\ w_{21} & w_{22} & \cdots & w_{3m} & b3 \end{bmatrix}$$

$\Downarrow$

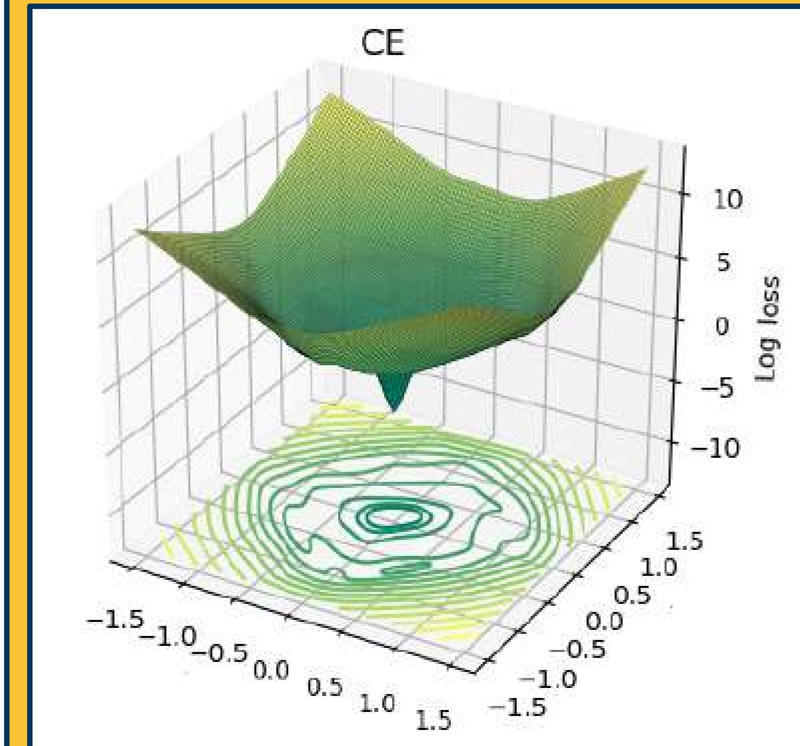
Loss

Optimization

As weights change, the loss changes as well

- This is often somewhat-smooth 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



Strategy: Follow the Slope!

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- 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

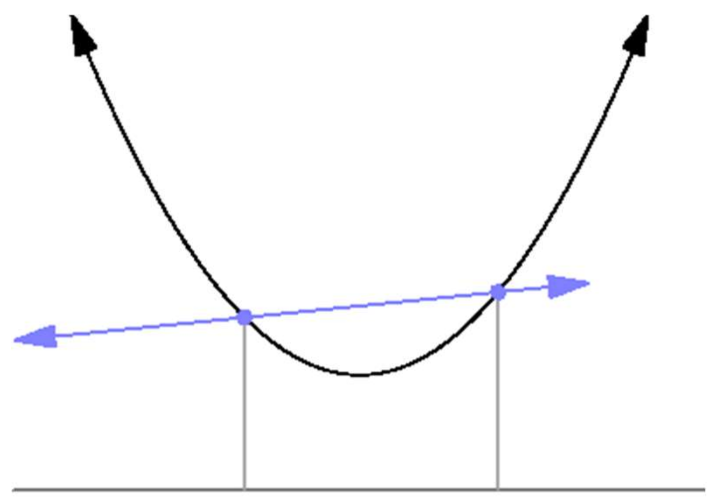


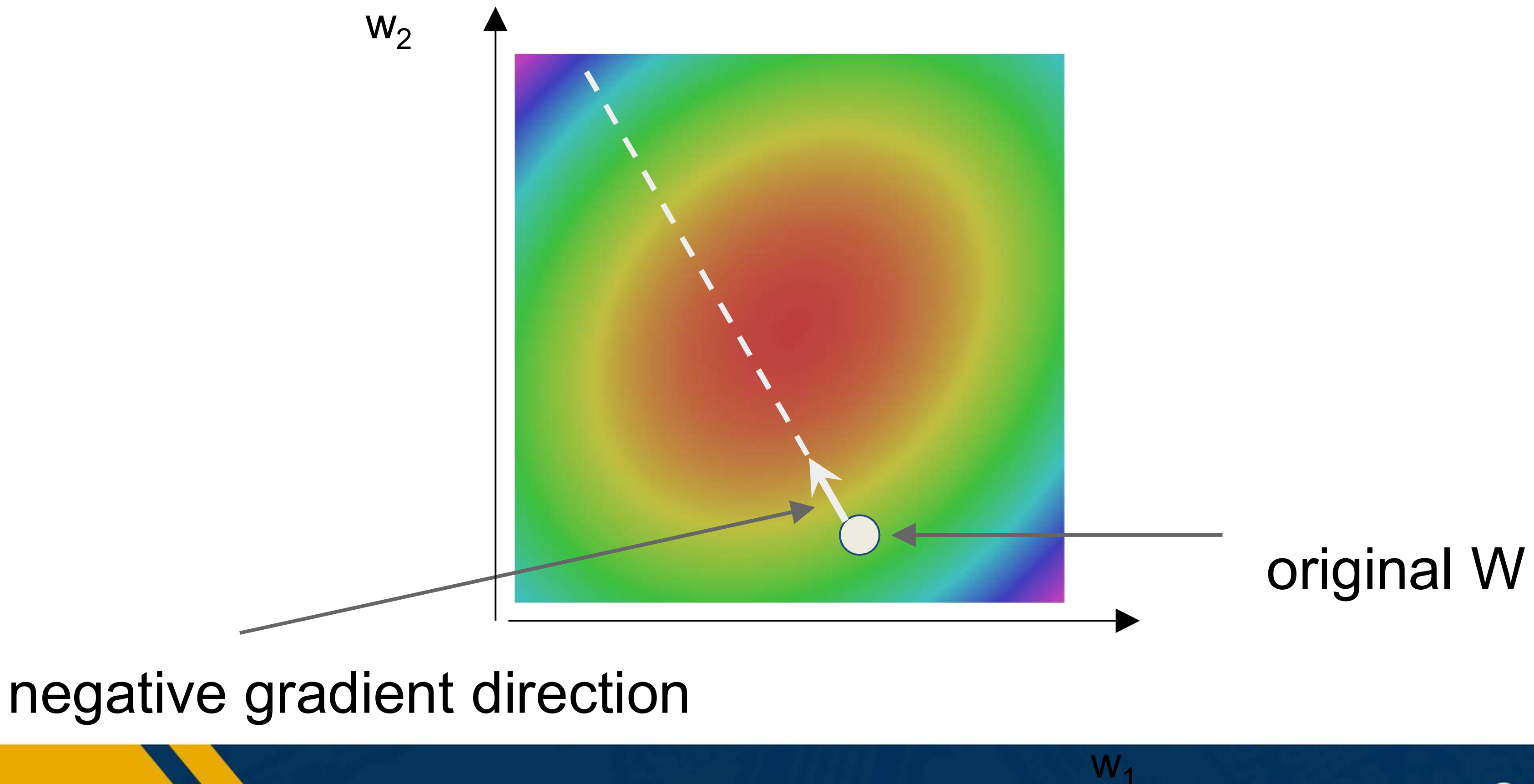
Image and equation from: https://en.wikipedia.org/wiki/Derivative#/media/File:Tangent_animation.gif

Derivatives

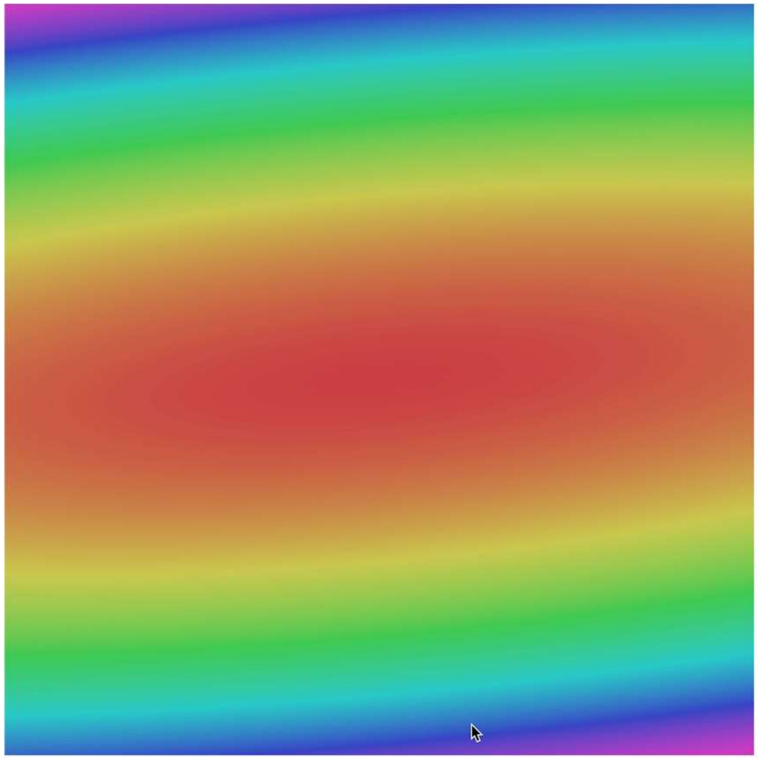
This idea can be turned into an **algorithm (gradient descent)**

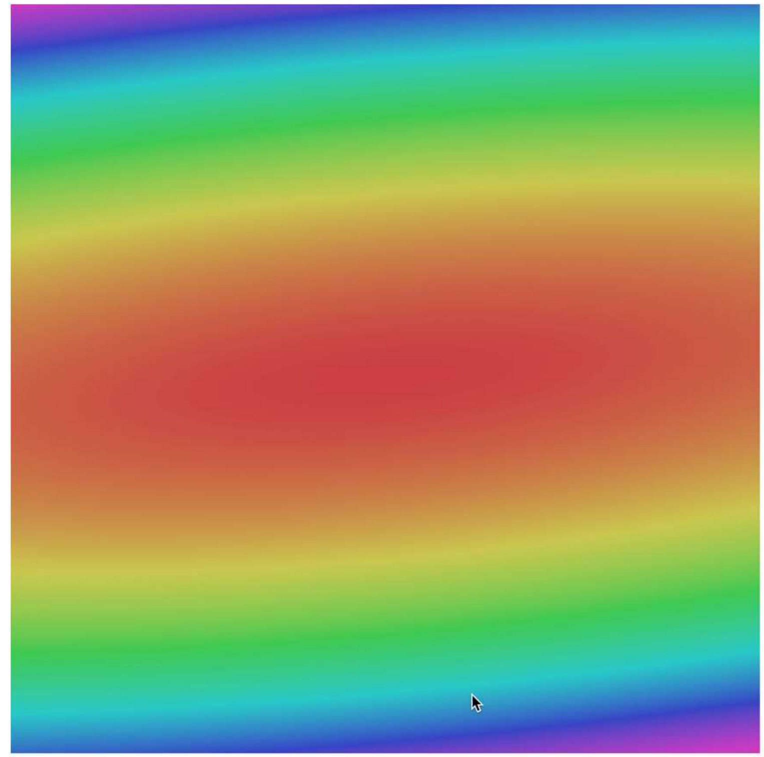
- Choose a model: $\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{W}) = \mathrm{Wx}$
- Choose loss function: $\boldsymbol{L_i} = |\boldsymbol{y} - \boldsymbol{W}\boldsymbol{x_i}|^2$
- Calculate partial derivative for each parameter: $\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{w_i}}$
- Update the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

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



Gradient Descent





w_1

Gradient Descent

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 $$L = \frac{1}{M}\sum L\left(f(x_i, W), y_i\right)$$
  - Where M is a *subset* of data
- We iterate over mini-batches:
  - Get mini-batch, compute loss, compute derivatives, and take a set

Mini-Batch Gradient Descent

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Gradient descent is guaranteed to converge under some conditions

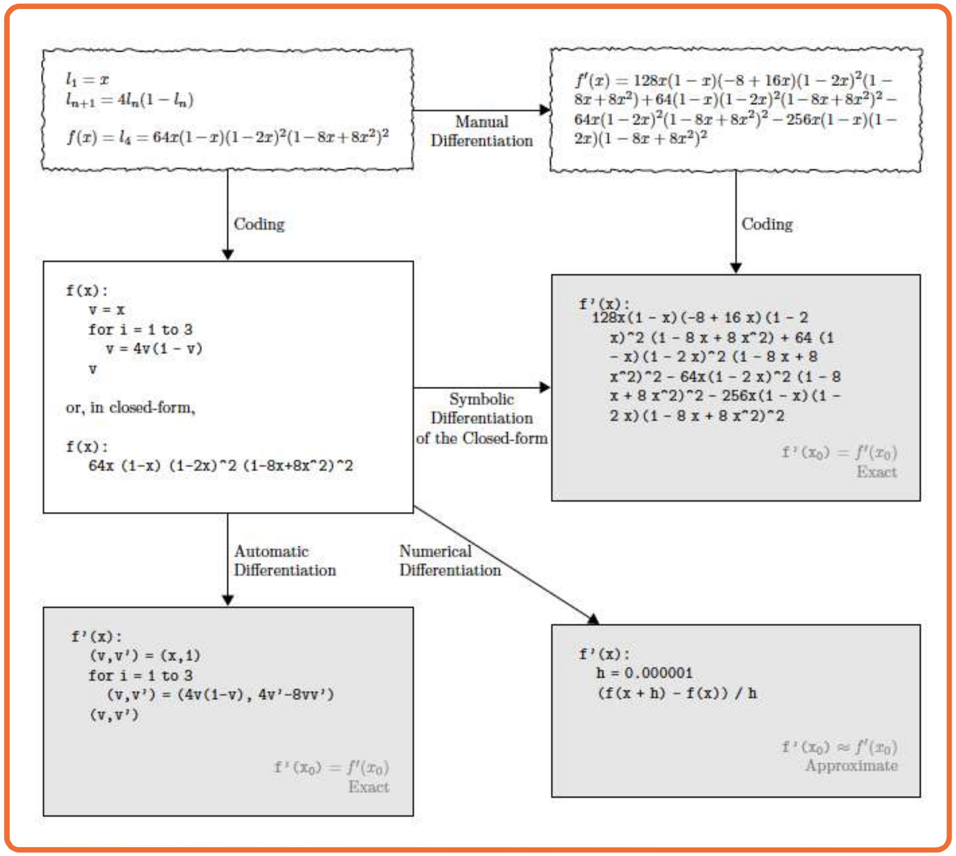
- For example, learning rate has to be appropriately reduced throughout training
- It will converge to a *local* minima
  - Small changes in weights would not decrease the loss
- It turns out that some of the local minima that it finds in practice (if trained well) are still pretty good!

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



current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

gradient dW:

[?,
?,
?,
?,
?,
?,
?,
?,
?,…]

current W:	**W + h** (first dim)**:**	**gradient dW:**
[0.34,	[0.34 + **0.0001**,	[?,
-1.11,	-1.11,	?,
0.78,	0.78,	?,
0.12,	0.12,	?,
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,	[0.34 + **0.0001**,	[**-2.5**,
-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**	

(1.25322 - 1.25347)/0.0001
= -2.5

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

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

current W:	**W + h** (second dim)**:**	**gradient dW:**
[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,…]	?,…]
loss 1.25347	**loss 1.25353**	

current W:	**W + h** (second dim)**:**	**gradient dW:**
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11 + **0.0001**,	**0.6**,
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 1.25353**	

(1.25353 - 1.25347)/0.0001
= 0.6

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

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

current W:	W + h (third dim):	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:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

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

gradient dW:

[-2.5,
0.6,
0,
?,
?,…]

(1.25347 - 1.25347)/0.0001
= 0

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

Numerical vs Analytic Gradients

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

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.**

For some functions, we can analytically derive the partial derivative

Example:

Function

$$f(w, x_i) = w^T x_i$$

Loss

$$(y_i - w^T x_i)^2$$

(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

For some functions, we can analytically derive the partial derivative

Example:

Function

$$f(w, x_i) = w^T x_i$$

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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 $\frac{\partial L}{\partial w_j}$?

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

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

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

…where… $\delta_k = y_k - w^T x_k$

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

$$= -2 \sum_{k=1}^{N} \delta_k x_{kj}$$

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

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

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

$$\mathrm{f(x)} = \sigma\left(\sum_k w_k x_k\right)$$

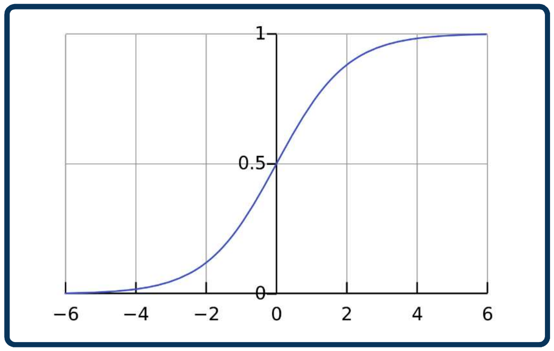
$$\mathrm{L} = \sum_i \left(y_i - \sigma\left(\sum_k w_k x_{ik}\right)\right)^2$$

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

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

$$= \sum_i -2\delta_i \sigma(\mathrm{d}_i)(1-\sigma(\mathrm{d}_i))x_{ij}$$

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



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 $\sigma_i = \sigma\left(\sum_{j=1}^{m} w_j x_{ij}\right)$

$$\delta_i = y_i - \sigma_i$$

Adding a Non-Linear Function

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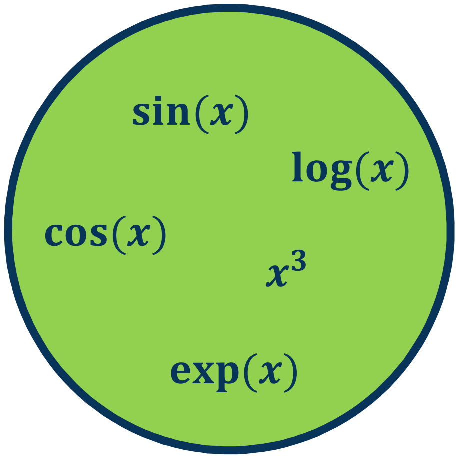
Decomposing a Function

Given a library of simple functions



Compose into a complicate function

$$-\log\left(\frac{1}{1+e^{-w\cdot x}}\right)$$

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

Linear Algebra View: Vector and Matrix Sizes

Georgia Tech

$$\begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} & b1 \\ w_{21} & w_{22} & \cdots & w_{2m} & b2 \\ w_{31} & w_{32} & \cdots & w_{3m} & b3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \\ 1 \end{bmatrix}$$

W $\quad$ x

Sizes: $[c \times (d+1)]$ $\quad$ $[(d+1) \times 1]$

Where c is number of classes

d is dimensionality of input

Closer Look at a Linear Classifier

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Conventions:

- Size of derivatives for scalars, vectors, and matrices: Assume we have scalar $\boldsymbol{s} \in \mathbb{R}^{\mathbf{1}}$, vector $\boldsymbol{v} \in \mathbb{R}^{\boldsymbol{m}}$, i.e. $\boldsymbol{v} = [\boldsymbol{v_1}, \boldsymbol{v_2}, \ldots, \boldsymbol{v_m}]^{\boldsymbol{T}}$ and matrix $\boldsymbol{M} \in \mathbb{R}^{\boldsymbol{k \times \ell}}$

- What is the size of $\frac{\partial v}{\partial s}$? $\mathbb{R}^{\boldsymbol{m \times 1}}$ (column vector of size $\boldsymbol{m}$)

$$\begin{bmatrix} \frac{\partial v_1}{\partial s} \\ \frac{\partial v_2}{\partial s} \\ \vdots \\ \frac{\partial v_m}{\partial s} \end{bmatrix}$$

- What is the size of $\frac{\partial s}{\partial v}$? $\mathbb{R}^{\boldsymbol{1 \times m}}$ (row vector of size $\boldsymbol{m}$)

$$\begin{bmatrix} \frac{\partial s}{\partial v_1} & \frac{\partial s}{\partial v_1} & \cdots & \frac{\partial s}{\partial v_m} \end{bmatrix}$$

Conventions:

- What is the size of $\frac{\partial v^1}{\partial v^2}$? A matrix:

$$\begin{array}{c} \textbf{Col } j \\ \textbf{Row } i \quad \begin{bmatrix} \frac{\partial v_1^1}{\partial v_1^2} & \cdots & \cdots & \cdots & \cdots & \\ \cdots & & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \frac{\partial v_i^1}{\partial v_j^2} & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \end{bmatrix} \end{array}$$

- This matrix of partial derivatives is called a **Jacobian**

(Note this is slightly different convention than on Wikipedia)

Conventions:

- What is the size of $\frac{\partial s}{\partial M}$? A matrix:

$$\begin{bmatrix} \frac{\partial s}{\partial m_{[1,1]}} & \cdots & \cdots & \cdots & \cdots & \\ \cdots & & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \frac{\partial s}{\partial m_{[i,j]}} & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \end{bmatrix}$$

- What is the size of $\frac{\partial L}{\partial W}$?
  - Remember that loss is a **scalar** and W is a matrix:

$$\begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} & b1 \\ w_{21} & w_{22} & \cdots & w_{2m} & b2 \\ w_{31} & w_{32} & \cdots & w_{3m} & b3 \end{bmatrix}$$

Jacobian is also a matrix:

$$W$$

$$\begin{bmatrix} \frac{\partial L}{\partial w_{11}} & \frac{\partial L}{\partial w_{12}} & \cdots & \frac{\partial L}{\partial w_{1m}} & \frac{\partial L}{\partial b_1} \\ \frac{\partial L}{\partial w_{21}} & \cdots & \cdots & \frac{\partial L}{\partial w_{2m}} & \frac{\partial L}{\partial b_2} \\ \cdots & \cdots & \cdots & \frac{\partial L}{\partial w_{3m}} & \frac{\partial L}{\partial b_3} \end{bmatrix}$$

Dimensionality of Derivatives

Jacobians of Batches

Batches of data are **matrices** or **tensors** (multi-dimensional matrices)

Examples:

- Each instance is a vector of size m, our batch is of size $[\boldsymbol{B} \times \boldsymbol{m}]$
- Each instance is a matrix (e.g. grayscale image) of size $\boldsymbol{W} \times \boldsymbol{H}$, our batch is $[\boldsymbol{B} \times \boldsymbol{W} \times \boldsymbol{H}]$
- Each instance is a multi-channel matrix (e.g. color image with R,B,G channels) of size $\boldsymbol{C} \times \boldsymbol{W} \times \boldsymbol{H}$, our batch is $[\boldsymbol{B} \times \boldsymbol{C} \times \boldsymbol{W} \times \boldsymbol{H}]$

Jacobians become tensors which is complicated

- Instead, flatten input to a vector and get a vector of derivatives!
- This can also be done for partial derivatives between two vectors, two matrices, or two tensors

$$\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nn} \end{bmatrix}$$

Flatten

$$\begin{bmatrix} x_{11} \\ x_{12} \\ \vdots \\ x_{21} \\ x_{22} \\ \vdots \\ x_{n1} \\ \vdots \\ x_{nn} \end{bmatrix}$$