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

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

MISC

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

Recap:

Supervised Learning

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

Unsupervised Learning

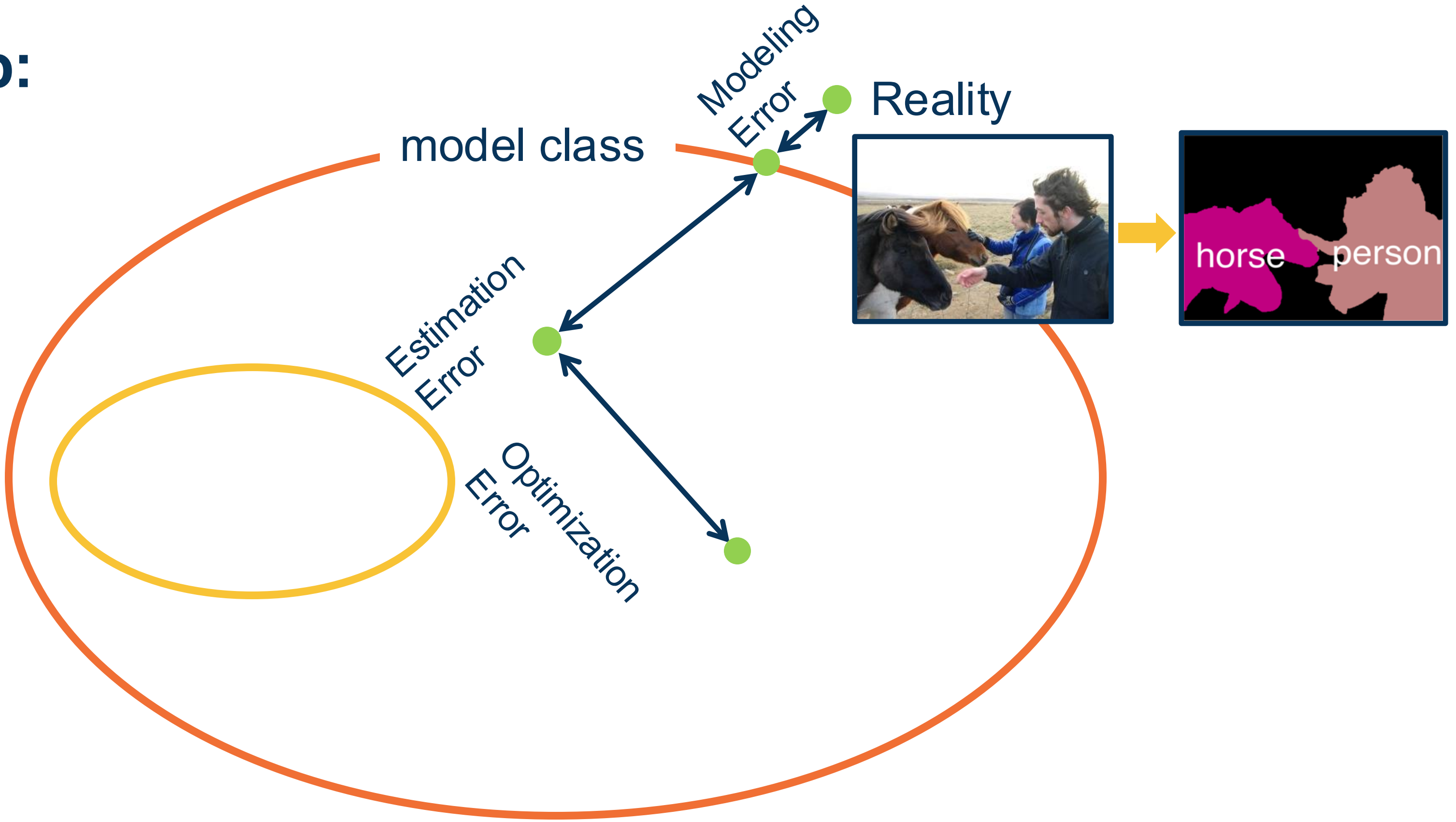
- Input: $\{X\}$
- Learning output: $P(x)$
- Example: Clustering, density estimation, etc.

Reinforcement Learning

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

Very often combined, sometimes within the same model!

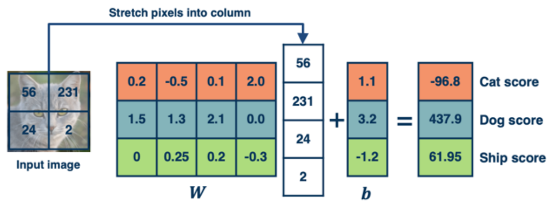
Recap:


Modeling Error
Reality
model class
horse
person
Estimation Error
Optimization Error

Recap:

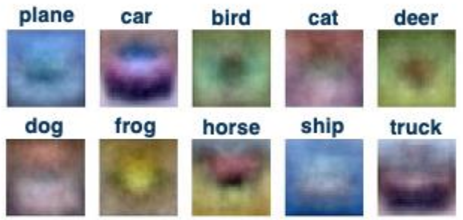
Algebraic Viewpoint

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



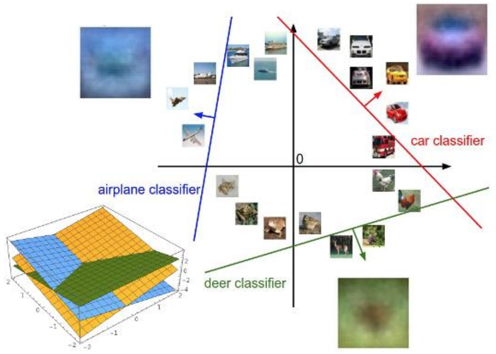
Visual Viewpoint

One template per class



Geometric Viewpoint

Hyperplanes cutting up space



Adapted from from CS 231n slides

This time:

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

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

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

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

SVM Loss Example

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**
	High Loss	Low Loss	High Loss

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

Given a dataset of examples:

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

Where x_i is image and

y_i is (integer) label

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

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

Adapted from from CS 231n slides

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: $\boldsymbol{s_i = f(x_i, W)}$

the SVM loss has the form:

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

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

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

$$\boldsymbol{y_i = 0}$$

cat	**3.2**	$\boldsymbol{s_{j=0} = s_{y_i}}$	
car	3.1	$\boldsymbol{s_{j=1}}$	$\max(0, 3.1 - 3.2 + 1)$
frog	1.7	$\boldsymbol{s_{j=2}}$	$\max(0, 1.7 - 3.2 + 1)$

$$L = 0.9 + 0 = 0.9$$

Multiclass SVM loss:

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

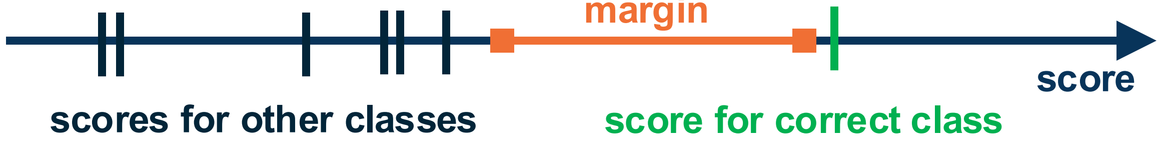
and using the shorthand for the scores vector: $s = f(x_i, W)$

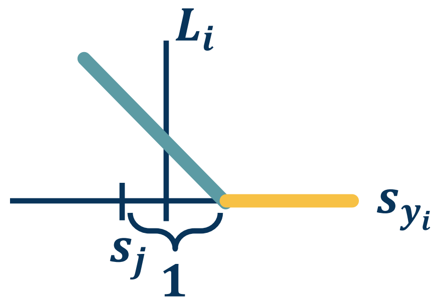
the SVM loss has the form:

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

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

Loss = 0:





Performance Measure for Scores

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:

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

= 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 from CS 231n slides

SVM Loss Example

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:

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

= 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	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	**0.0**	

Adapted from from CS 231n slides

SVM Loss Example

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:

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

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:

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

Adapted from from CS 231n slides

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 (e.g., $\pm$ 0.1)?

No change for small values

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**

Adapted from from CS 231n slides

SVM Loss Example

Multiclass SVM loss:

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

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

Q: What is min/max of loss value?

[0,inf]

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

Adapted from from CS 231n slides

SVM Loss Example

Multiclass SVM loss:

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

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

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

num_class - 1

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

Adapted from from CS 231n slides

SVM Loss Example

Georgia Tech

Multiclass SVM loss:

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

Q: What if we used mean instead of sum?

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**

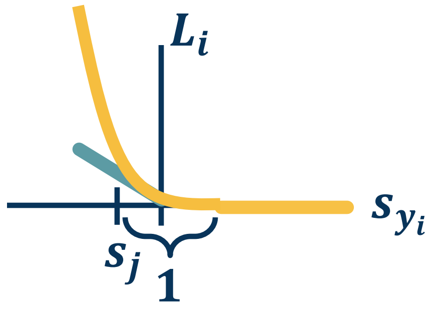
Adapted from from CS 231n slides

SVM Loss Example

Multiclass SVM loss:

$$L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)^2$$

Q: What if we used **squared** hinge loss?



- Smooth loss around hinge
- Sensitive to outliers (larger penalty)

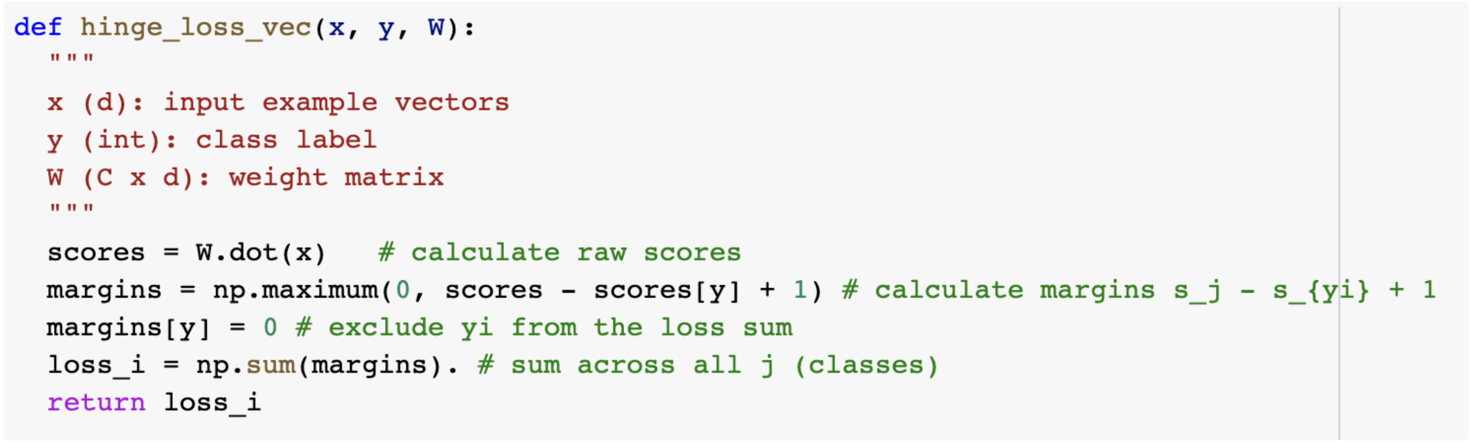
Suppose: 3 training examples, 3 classes.
With some $\boldsymbol{W}$ the scores $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{W})=\boldsymbol{W}\boldsymbol{x}$ are:

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

Adapted from from CS 231n slides

Multiclass SVM loss:

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



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

Adapted from from CS 231n slides

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

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

E.g. Suppose that we found a W such that L = 0.

Q: Is this W unique?

Let’s look at an example

Adapted from from CS 231n slides

SVM Loss Example

Georgia Tech

Multiclass SVM loss:

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**

Before:
= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

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

Adapted from from CS 231n slides

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

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

E.g. Suppose that we found a W such that L = 0.

Q: Is this W unique?

No, 2W also has L=0

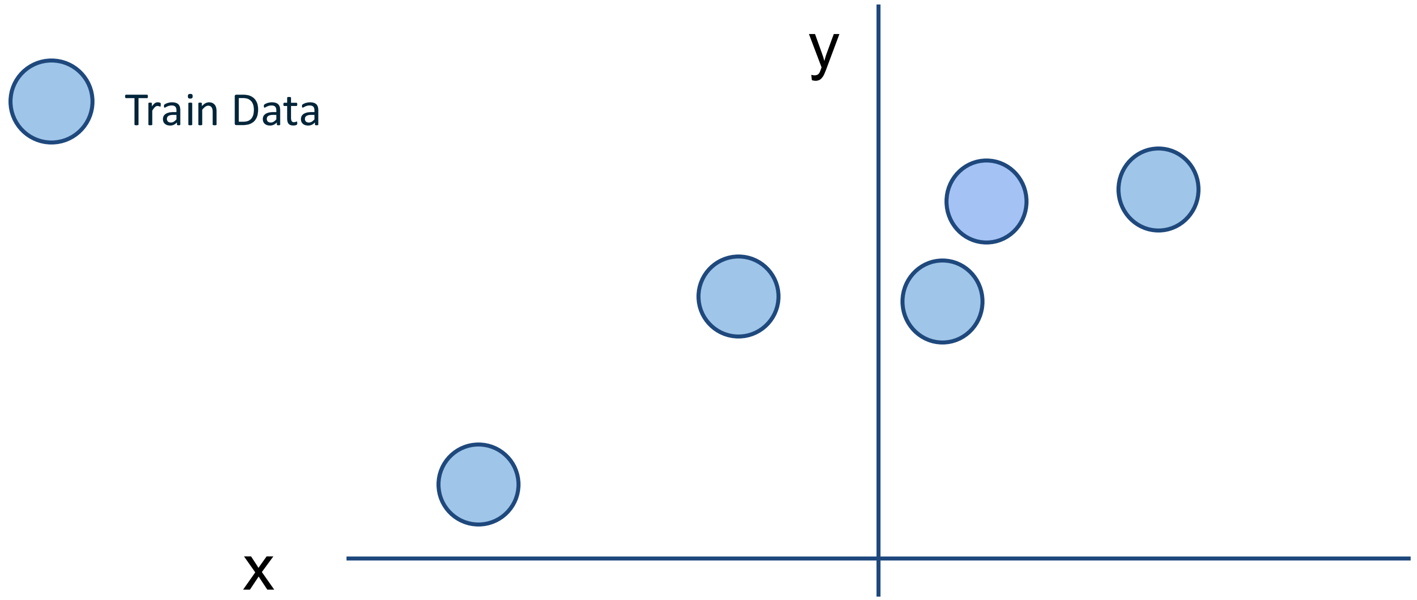
How do we choose between W, 2W, and 1e+7W?

Adapted from from CS 231n slides

SVM Loss Example

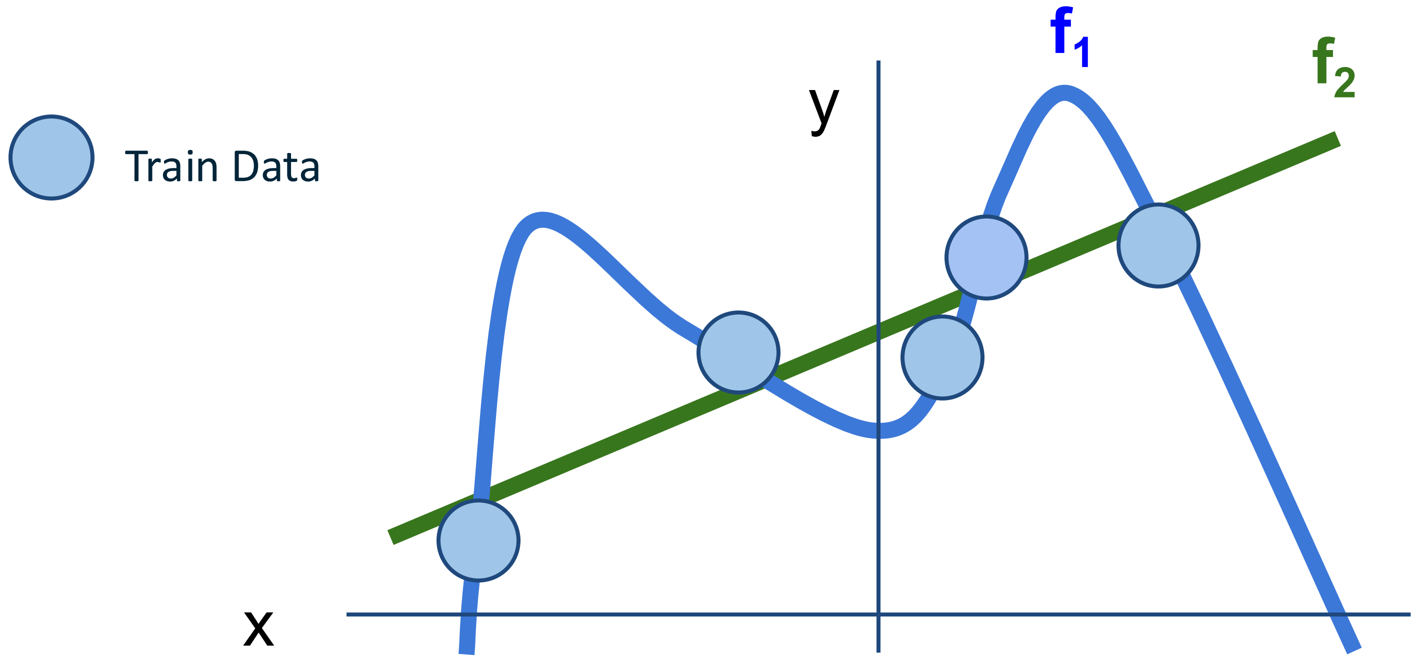
Georgia Tech

Regularization intuition: fitting a polynomial function



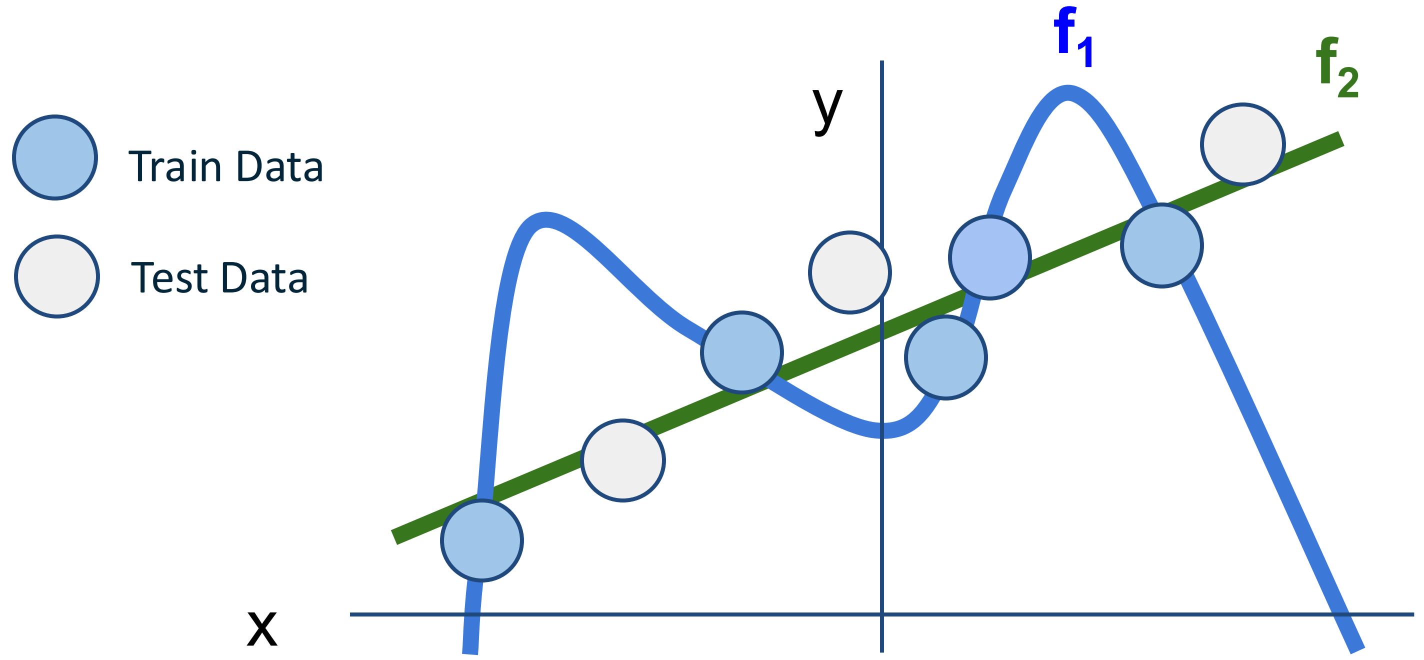
Adapted from from CS 231n slides

Regularization intuition: fitting a polynomial function



Adapted from from CS 231n slides

Regularization intuition: fitting a polynomial function



Regularization balances the simplicity of the function and loss, so we don't overfit to the noises in the data

Adapted from from CS 231n slides

Regularization

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss: Model predictions should match training data}} + \underbrace{\lambda R(W)}_{\text{Regularization: Prevent the model from doing too well on training data}}$$

Data loss: Model predictions should match training data

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

Adapted from from CS 231n slides

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

Regularization

λ = regularization strength (hyperparameter)

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

Data loss: Model predictions should match training data

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

Simple examples

<u>L2 regularization:</u> $R(W) = \sum_k \sum_l W_{k,l}^2$

L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$

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

More complex (DNN-specific):

Dropout

Batch/layer normalization

Stochastic depth, fractional pooling, etc

Regularization: Implement a simple L2 regularizer

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

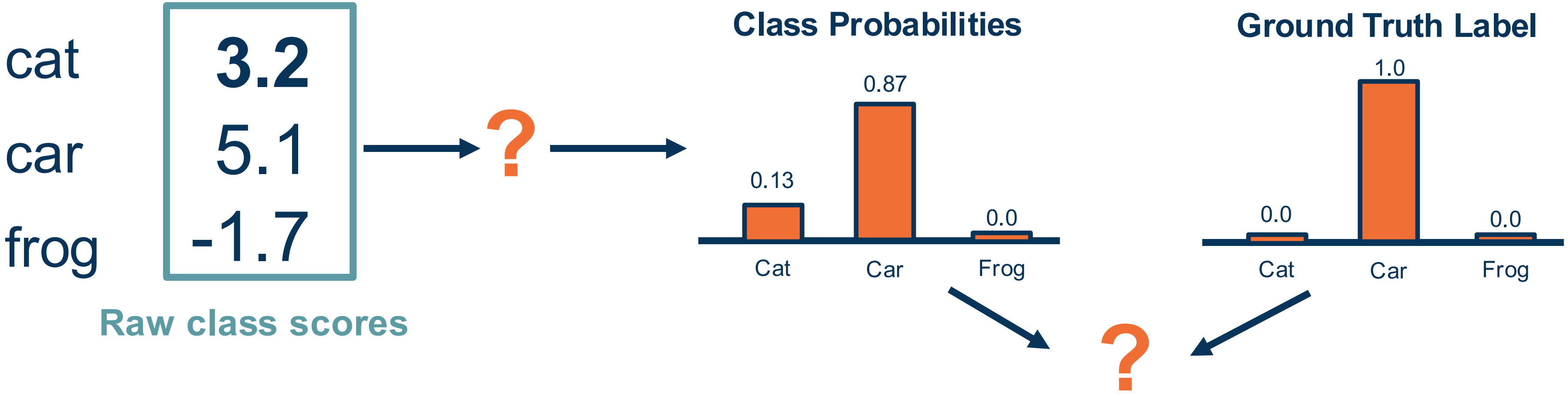
```
def l2_regularized_hinge_loss(x, y, W, reg_coeff):
  data_loss = 0
  # calculate dataset loss
  for i in range(x.shape[0]):
    data_loss += hinge_loss_vec(x[i], y[i], W)

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

  return data_loss + reg_loss
```

What if we want probabilities?

We need a different classifier and a way to compute loss on probability (mismatch)!*



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

Softmax Classifier (Multinomial Logistic Regression)

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

$$\boxed{s = f(x_i; \theta)}$$

Probabilities must be >= 0

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

Softmax Function

Probabilities must sum to 1

	Unnormalized log-probabilities / logits		Unnormalized probabilities		Probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1	$\xrightarrow{\text{exp}}$	164.0	$\xrightarrow{\text{normalize}}$	0.87
frog	-1.7		0.18		0.00

How do we compute the loss?

Adapted from from CS 231n slides

Softmax Classifier (Multinomial Logistic Regression)

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

$$\boxed{\boldsymbol{s = f(x_i; \theta)}}$$

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

Softmax Function

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

	Unnormalized log-probabilities / logits		Predicted Probs (softmax)
cat	**3.2**	$\xrightarrow{\text{softmax}}$	**0.13**
car	5.1		0.87
frog	-1.7		0.00

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

This is equivalent to:

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

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

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

Softmax Classifier (Multinomial Logistic Regression)

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

$$\boxed{s = f(x_i; \theta)}$$

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

Softmax Function

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

	Unnormalized log-probabilities / logits	Predicted Probs (softmax)
cat	3.2	0.13
car	5.1	0.87
frog	-1.7	0.00

$\xrightarrow{\text{softmax}}$

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

This is equivalent to:

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

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

Negative Log Likelihood (NLL)

Cross-Entropy Loss Example

Softmax Classifier (Multinomial Logistic Regression)

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

$$\boxed{s = f(x_i; \theta)}$$

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

Softmax Function

2. Information theory view

cat	**3.2**	softmax	**0.13**	**1.00**
car	5.1		0.87	0.00
frog	-1.7		0.00	0.00

$$\text{logits} \xrightarrow{\text{softmax}} \text{predicted probs} \rightarrow \text{maximize agreement} \leftarrow \text{correct probs}$$

Unnormalized log-probabilities / logits

Predicted Probs (softmax)

Correct probs

Adapted from from CS 231n slides

Softmax Classifier (Multinomial Logistic Regression)

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

$$\boxed{s = f(x_i; \theta)}$$

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

Softmax Function

2. Information theory view

cat	**3.2**	$\xrightarrow{\text{softmax}}$	**0.13**	1.00
car	5.1		0.87	0.00
frog	-1.7		0.00	0.00

Unnormalized log-probabilities / logits — **Predicted Probs (softmax)** $\rightarrow$ maximize agreement $\leftarrow$ **Correct probs**

Cross Entropy: $H(p,q) = -\sum p(x) \ln q(x)$

Cross Entropy Loss -> NLL

$$H_i(p, p_\theta) = -\sum_{y \in Y} p(y|x_i) \ln p_\theta(y|x_i)$$
$$= -\ln p_\theta(y_i|x_i)$$

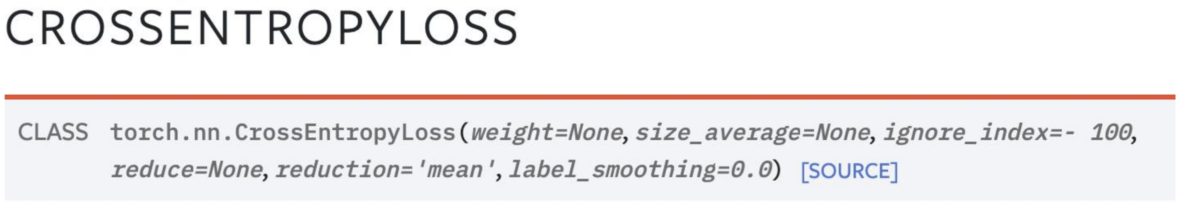
$$L = \sum H_i(p, p_\theta) = -\sum \ln p_\theta(y_i|x_i) \equiv NLL$$

Adapted from from CS 231n slides

Cross-Entropy Loss Example

Softmax Classifier (Multinomial Logistic Regression)

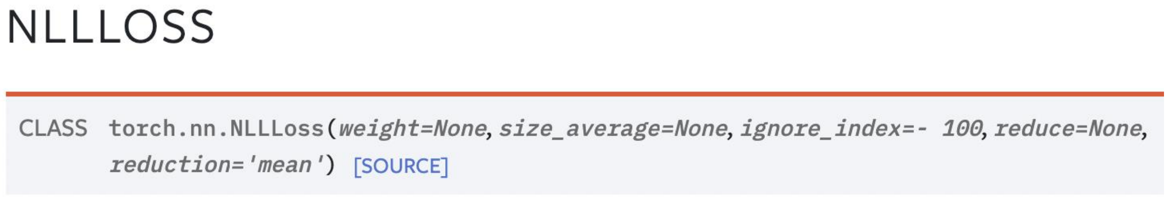
NLL and CrossEntropy are different loss functions in PyTorch!



CROSSENTROPYLOSS

CLASS `torch.nn.CrossEntropyLoss(`*`weight=None, size_average=None, ignore_index=- 100, reduce=None, reduction='mean', label_smoothing=0.0`*`)` [SOURCE]

Expects unformalized logits as input (the function will apply softmax & log on top)



NLLLOSS

CLASS `torch.nn.NLLLoss(`*`weight=None, size_average=None, ignore_index=- 100, reduce=None, reduction='mean'`*`)` [SOURCE]

Expects log probabilities as input (do softmax yourself!)

Softmax Classifier (Multinomial Logistic Regression)

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

$$\boxed{\boldsymbol{s = f(x_i;\theta)}}$$

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

Softmax Function

Cross-entropy loss:

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

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

Infimum is 0, max is unbounded (inf)

As $p_\theta(y_i, x_i) \rightarrow 0,\ L \rightarrow \inf$

Adapted from from CS 231n slides

Softmax Classifier (Multinomial Logistic Regression)

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

$$\boxed{\boldsymbol{s = f(x_i; \theta)}}$$

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

Softmax Function

Cross-entropy loss:

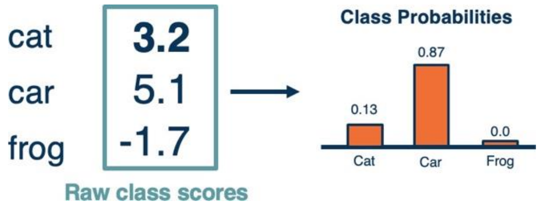
$$L_i = -\log(p_\theta(y_i|x_i))$$

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

-log(1/C), e.g. -log(1/3)=log(3) ≈ 1.1

Adapted from from CS 231n slides

Q: Why softmax?



Why this?

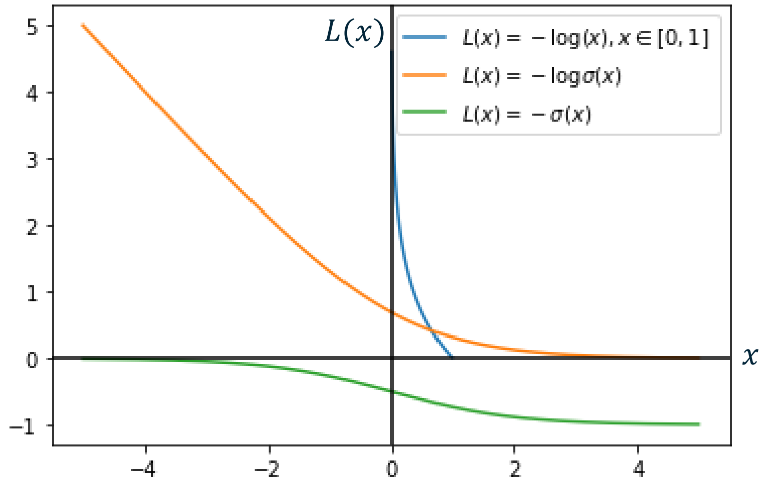
$$\boxed{p_\theta(Y = y_i | X = x_i) = \frac{e^{s_{y_i}}}{\sum_j e^{s_j}}}$$

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

$$: (;\ ) = \frac{<\%}{1 + <\%}$$

Consider the following three basis for NLL:

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



Problem with Squash and clip?

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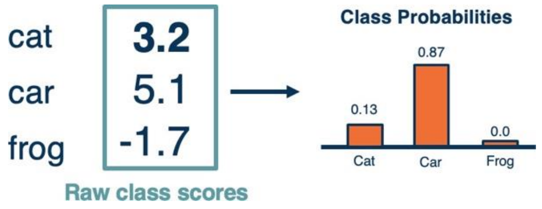

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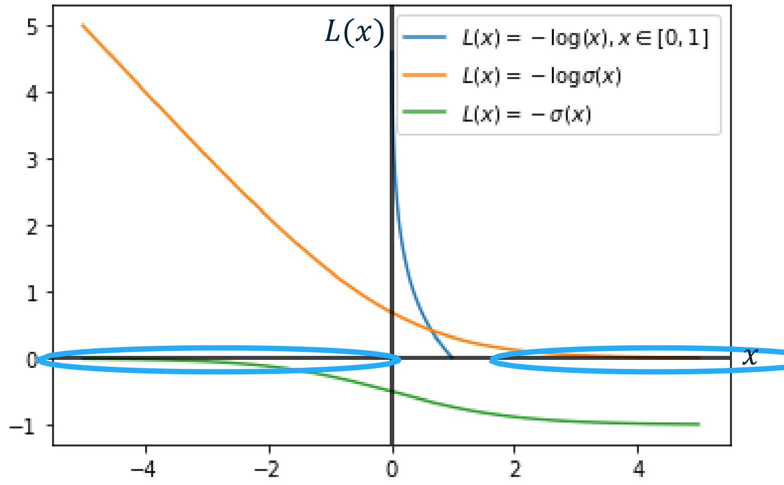
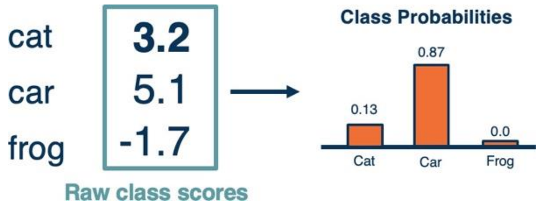


Problem with Squash and clip?

No loss, no learning!

Q: Why softmax?



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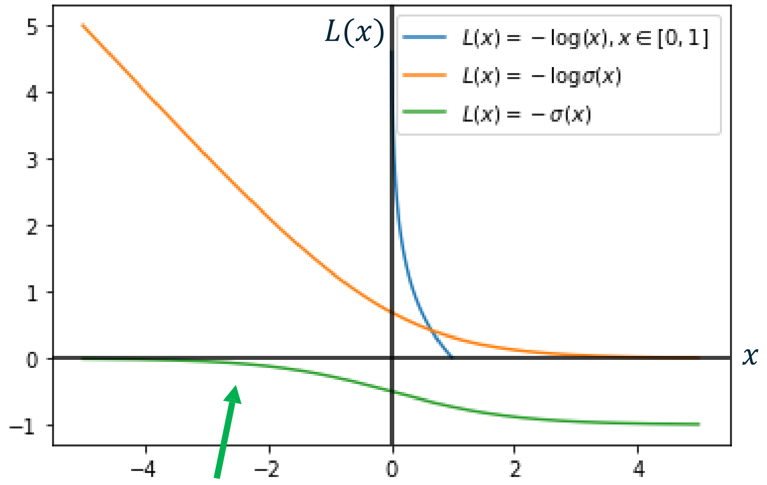
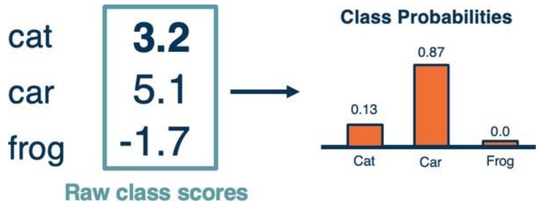


2. Negative likelihood w/ logistic function: saturated loss when classifier is very wrong

Q: Why softmax?



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

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

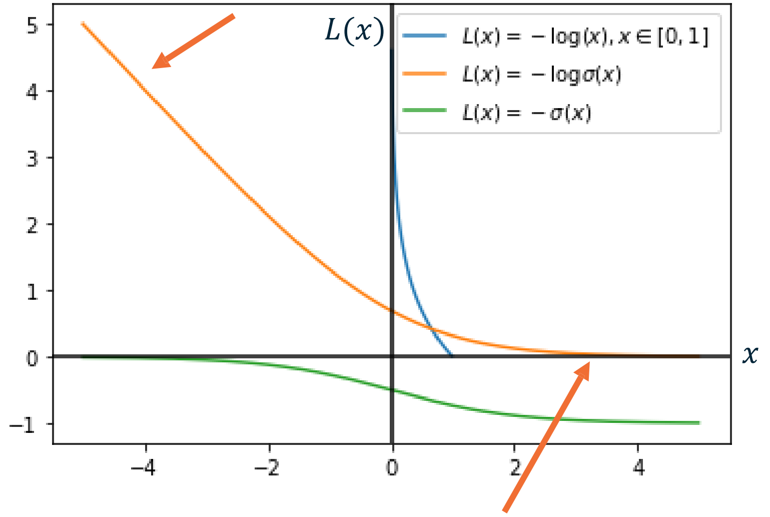
$$: (;\ ) = \frac{<\%}{1 + <\%}$$

Consider the following three basis for NLL:

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

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

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



Only saturate at convergence, e.g. $\sigma(3) \approx 0.95$

So, what is a loss function?

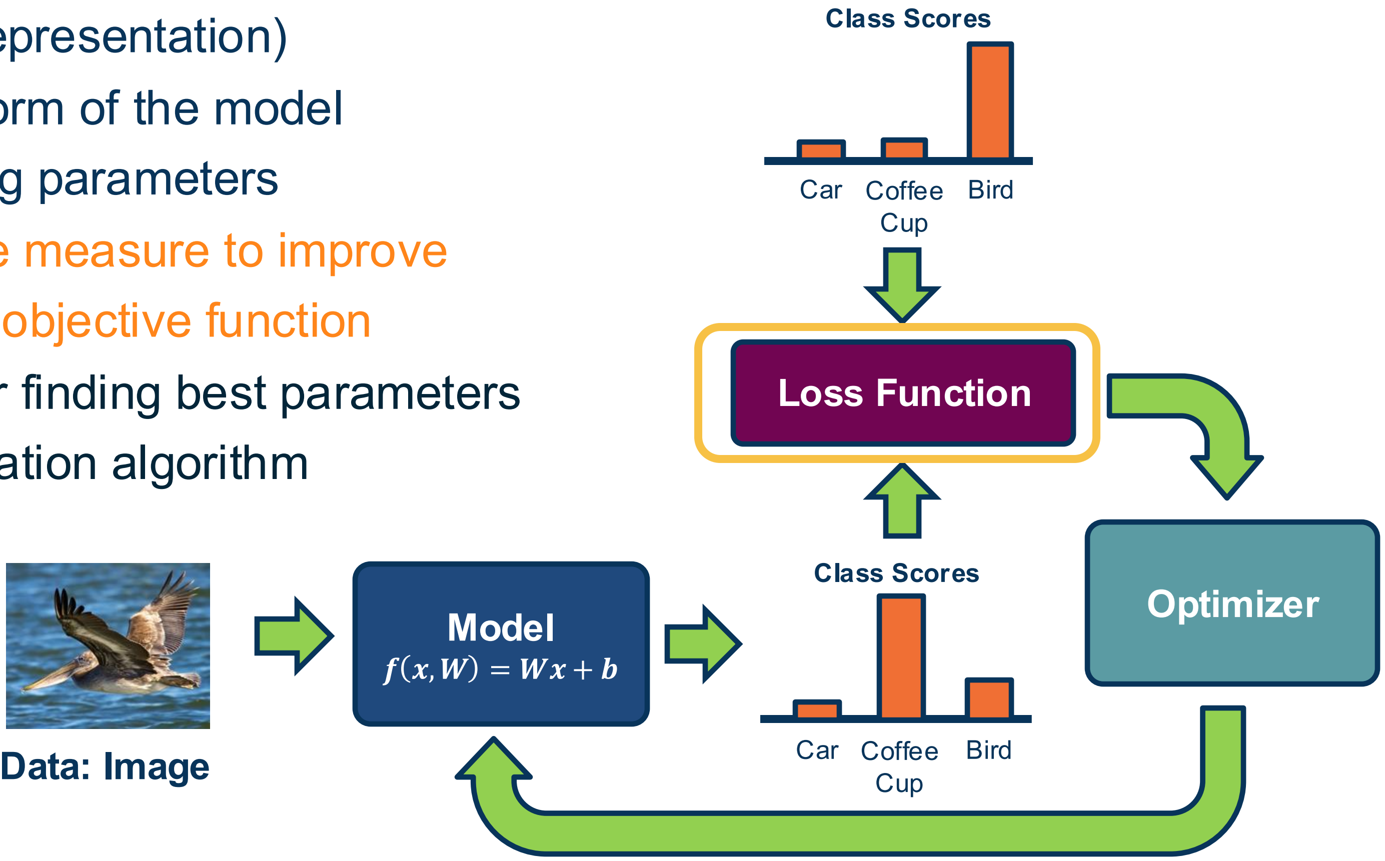
- In this context, it’s a function that scores how well a **model** performs on a task. We often focus on the parameters rather than the hypothesis class.
- If $L(\theta_1, data) < L(\theta_2, data)$, then θ_1 is considered better.

- **Losses** are different than **metrics.** Loss functions are designed for optimization, which require properties like differentiability and smoothness.
- Example: CrossEntropy is a loss function for the multi-class classification task. Classification accuracy (how often the model is correct) is the metric.
- Losses can be used as metrics but are often not very interpretable.
- Losses can always be used as metrics, but metrics often cannot be used as loss functions (e.g., classification accuracy is not differentiable).

Summary: SVM and Softmax Classifier

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

- 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



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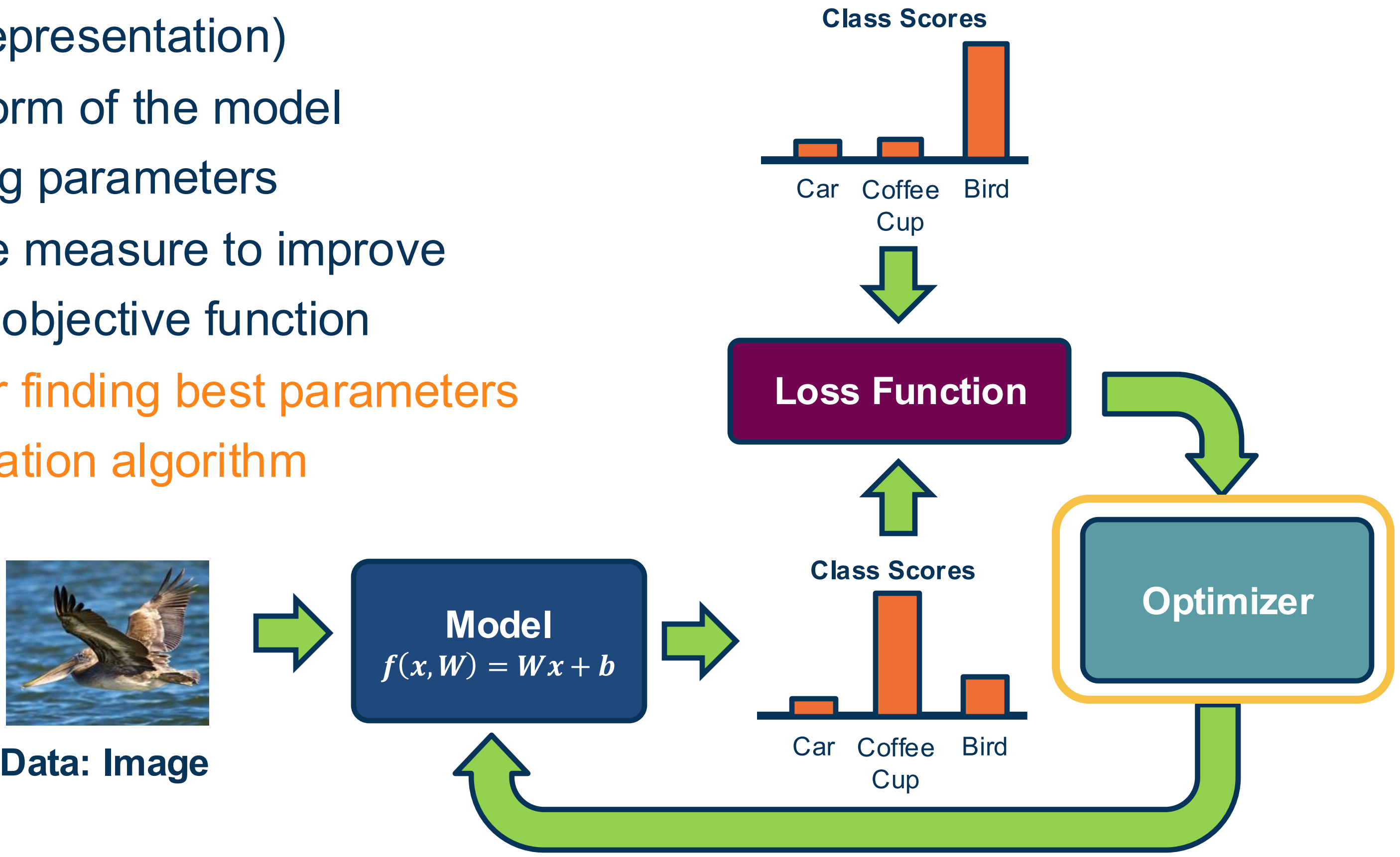
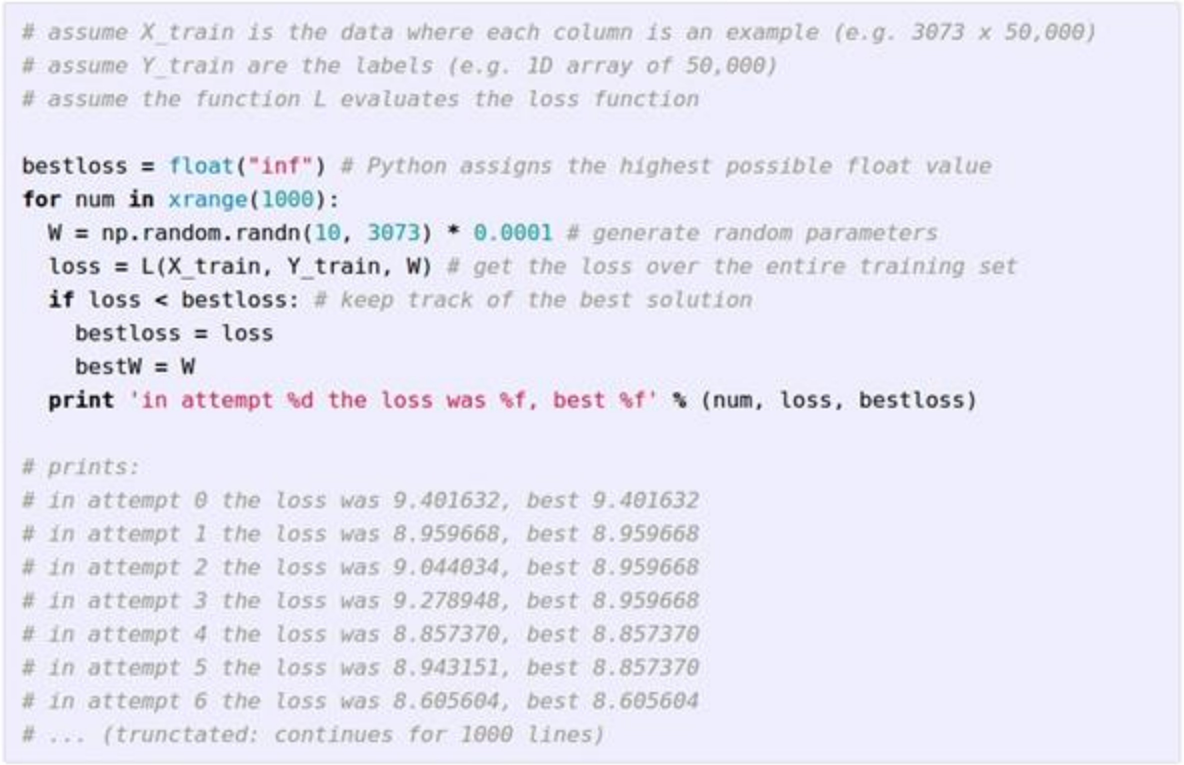


Strategy #1: A first very bad idea solution: **Random search**

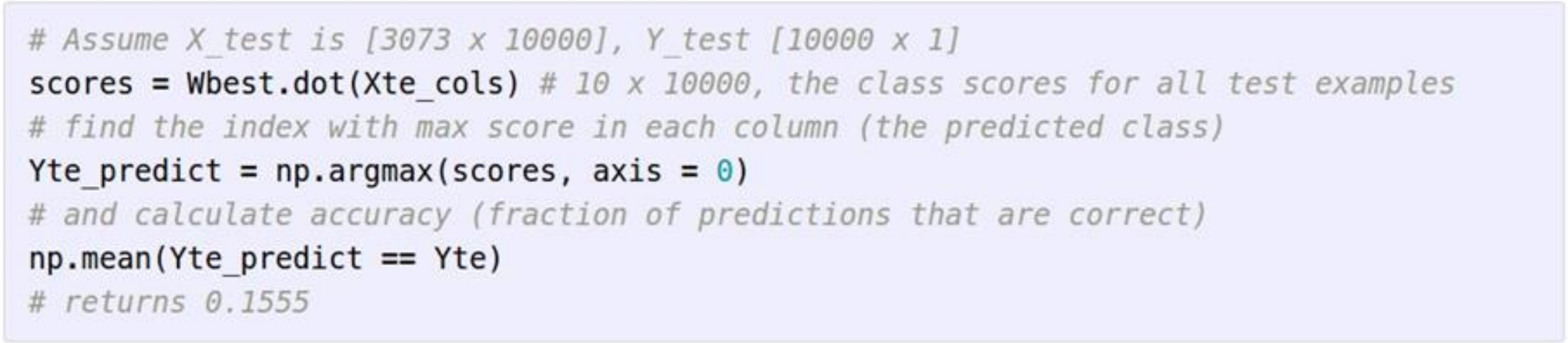


```
# assume X_train is the data where each column is an example (e.g. 3073 x 50,000)
# assume Y_train are the labels (e.g. 1D array of 50,000)
# assume the function L evaluates the loss function

bestloss = float("inf") # Python assigns the highest possible float value
for num in xrange(1000):
  W = np.random.randn(10, 3073) * 0.0001 # generate random parameters
  loss = L(X_train, Y_train, W) # get the loss over the entire training set
  if loss < bestloss: # keep track of the best solution
    bestloss = loss
    bestW = W
  print 'in attempt %d the loss was %f, best %f' % (num, loss, bestloss)

# prints:
# in attempt 0 the loss was 9.401632, best 9.401632
# in attempt 1 the loss was 8.959668, best 8.959668
# in attempt 2 the loss was 9.044034, best 8.959668
# in attempt 3 the loss was 9.278948, best 8.959668
# in attempt 4 the loss was 8.857370, best 8.857370
# in attempt 5 the loss was 8.943151, best 8.857370
# in attempt 6 the loss was 8.605604, best 8.605604
# ... (trunctated: continues for 1000 lines)
```

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



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

15.5% accuracy! not bad!
(SOTA is ~99.7%)

Adapted from from CS 231n slides

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

- Find the best combination of weights that minimizes our loss function

Several classes of methods:

- Random search
- Genetic algorithms (population-based search)
- Gradient-based optimization

In deep learning, **gradient-based methods are dominant** although not the only approach possible

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

Loss

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

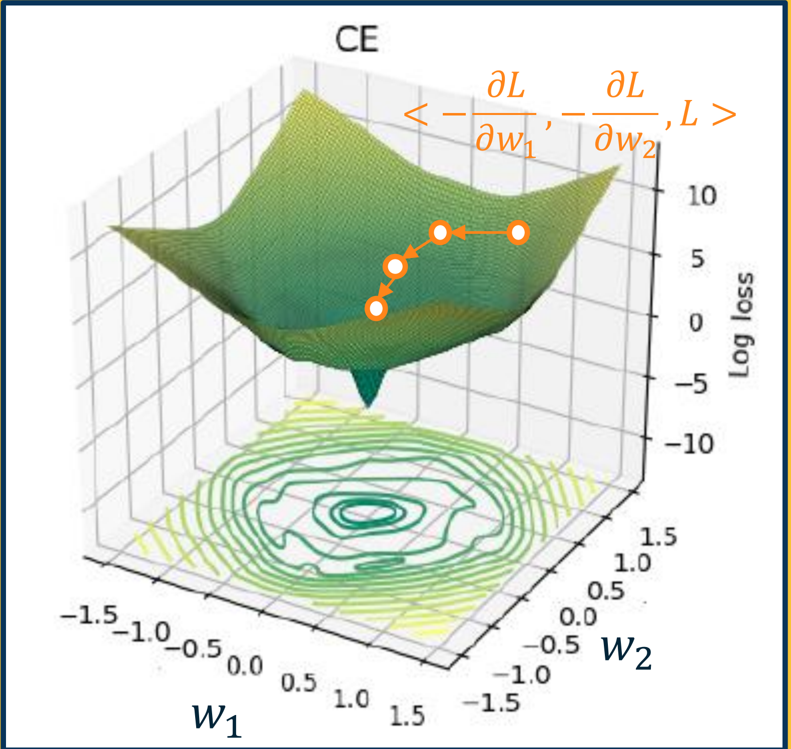
Optimization

Gradient Descent: Follow the Slope!

As weights change, the gradients change 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



- We can find the steepest descent direction by computing the **derivative:**

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

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

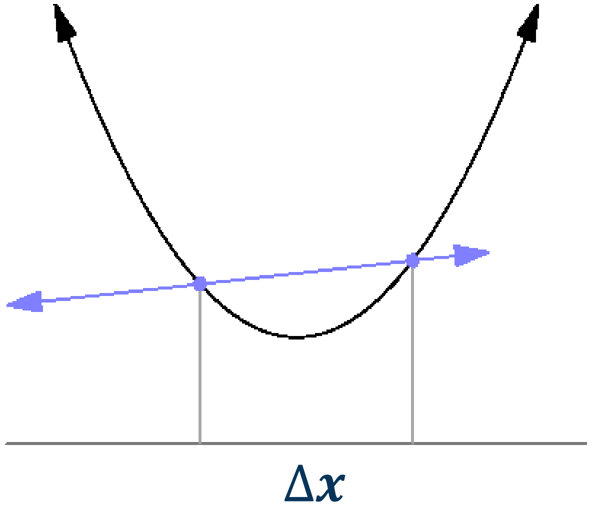


Image and equation from: https://en.wikipedia.org/wiki/Derivative #/media/File:Tangent_animation.gif

Derivatives

Calculate gradients: finite differences

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

Calculate gradients: finite differences

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**	

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

Calculate gradients: finite differences

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

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

Calculate gradients: finite differences

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**	

Calculate gradients: finite differences

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 (second dim):

[0.34,
-1.11 + **0.0001**,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25353

gradient dW:

[-2.5,
0.6,
?,
?,
?,…]

(1.25353 - 1.25347)/0.0001
= 0.6

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

Calculate gradients: finite differences

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**	

Calculate gradients: finite differences

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**,
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**	

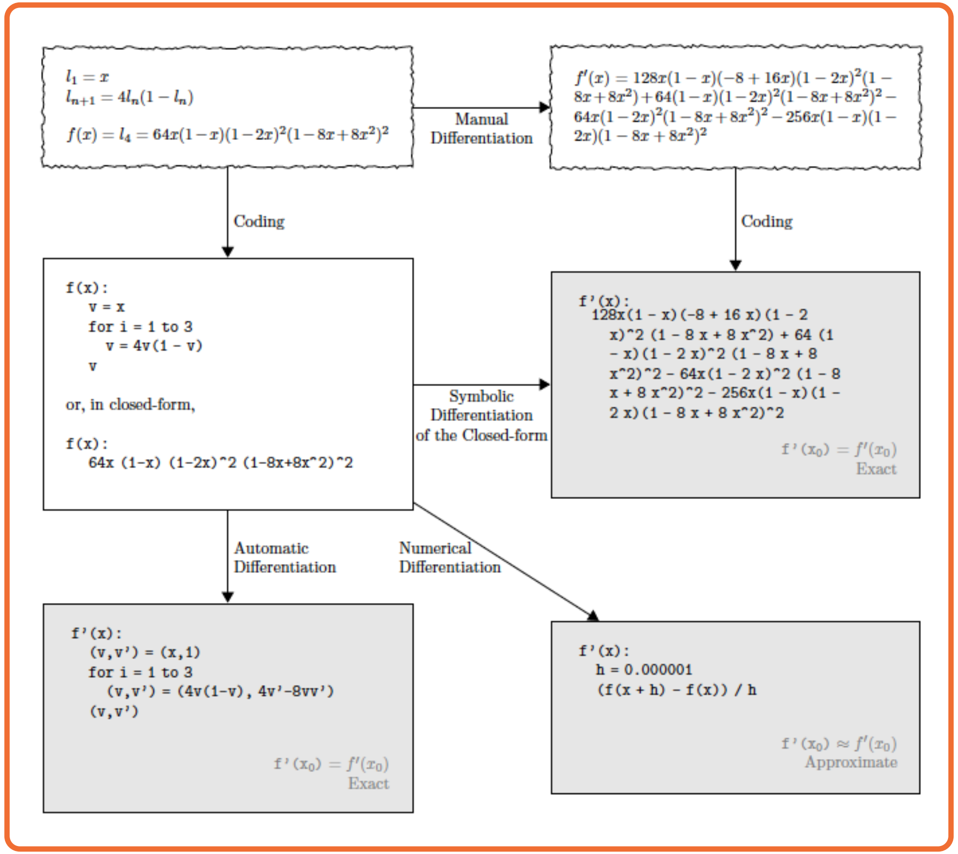
(1.25347 - 1.25347)/0.0001
= 0

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

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

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

More on **autodiff**:
https://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/readings/L06%20Automatic%20Differentiation.pdf



Manual Differentiation
Coding
Coding
Symbolic Differentiation of the Closed-form
Automatic Differentiation
Numerical Differentiation

$l_1 = x$
$l_{n+1} = 4l_n(1-l_n)$
$f(x) = l_4 = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$

$f'(x) = 128x(1-x)(-8+16x)(1-2x)^2(1-8x+8x^2) + 64(1-x)(1-2x)^2(1-8x+8x^2)^2 - 64x(1-2x)^2(1-8x+8x^2)^2 - 256x(1-x)(1-2x)(1-8x+8x^2)^2$

```
f(x):
  v = x
  for i = 1 to 3
    v = 4v(1 - v)
  v
```

or, in closed-form,

```
f(x):
  64x (1-x) (1-2x)^2 (1-8x+8x^2)^2
```

```
f'(x):
 128x(1 - x)(-8 + 16 x)(1 - 2
   x)^2 (1 - 8 x + 8 x^2) + 64 (1
   - x)(1 - 2 x)^2 (1 - 8 x + 8
   x^2)^2 - 64x(1 - 2 x)^2 (1 - 8
   x + 8 x^2)^2 - 256x(1 - x)(1 -
   2 x)(1 - 8 x + 8 x^2)^2
```

f'$(x_0) = f'(x_0)$
Exact

```
f'(x):
  (v,v') = (x,1)
  for i = 1 to 3
    (v,v') = (4v(1-v), 4v'-8vv')
  (v,v')
```

f'$(x_0) = f'(x_0)$
Exact

```
f'(x):
  h = 0.000001
  (f(x + h) - f(x)) / h
```

f'$(x_0) \approx f'(x_0)$
Approximate

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 implement
Analytic gradient: fast, exact, error-prone if implemented by yourself

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

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

The gradient descent algorithm

- 1. Choose a model: $\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{W}) = \mathrm{Wx}$
- 2. Choose loss function: $\boldsymbol{L_i} = |\boldsymbol{y} - \boldsymbol{W}\boldsymbol{x_i}|^2$
- 3. Calculate partial derivative for each parameter: $\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{w_i}}$
- 4. Update the parameters: $\boldsymbol{w_i} = \boldsymbol{w_i} - \frac{\partial \boldsymbol{L}}{\partial \boldsymbol{w_i}}$
- 5. 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 3-5**

Gradient Descent on Softmax Classifier!

$$\xrightarrow{f_\theta}$$

	s	$\xrightarrow{\text{softmax}}$ $p = \frac{e^{s}}{\sum_j e^{s_j}}$	$\xrightarrow{\text{NLL}}$
cat	**3.2**	**0.13**	
car	5.1	0.87	0.886
frog	-1.7	0.00	

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

$$\downarrow$$

$$\frac{\partial L}{\partial s_i} = ?$$

Gradient Descent on Softmax Classifier!

$\xrightarrow{f_\theta}$

	s		p		
cat	**3.2**	$\xrightarrow{\text{softmax}}$	**0.13**	$\xrightarrow{\text{NLL}}$	0.886
car	5.1		0.87		
frog	-1.7		0.00		

$$p = \frac{e^{s}}{\sum_j e^{s_j}}$$

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

$$\downarrow$$

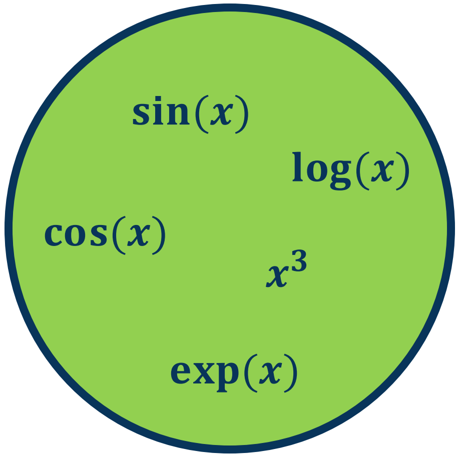
$$\frac{\partial L}{\partial s_{y_i}} = p_{y_i} - 1 \qquad \frac{\partial L}{\partial s_{j \neq y_i}} = p_j$$

$$\frac{\partial L}{\partial \theta} =? \longleftarrow \begin{matrix} \mathbf{-0.87} \\ 0.87 \\ 0.00 \end{matrix} \longleftarrow$$

$$\frac{\partial L}{\partial s}$$

$$\theta_i = \theta_i - \alpha \frac{\partial L}{\partial \theta_i}$$

Composing simple functions creates complex analytical gradients

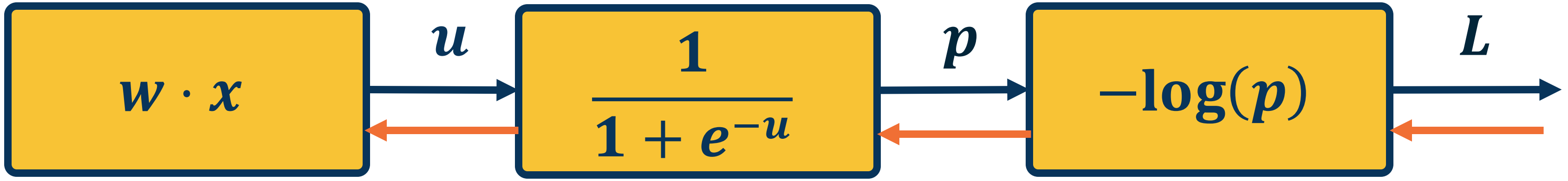


$$\xrightarrow[\text{complex function}]{\text{Compose into a}}$$

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

$$\begin{tikzcd}\boxed{w\cdot x} \arrow[r, "u"] & \boxed{\frac{1}{1+e^{-u}}} \arrow[r, "p"] & \boxed{-\log(p)} \arrow[r, "L"] & {}\end{tikzcd}$$

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



$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p}\frac{\partial p}{\partial u}\frac{\partial u}{\partial w}$$

Next time: Chain rule and Backpropagation!

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

Decomposing a Function

Georgia Tech