Lecture 3:
Loss function
Regularization
Optimization

Announcements (also on Piazza)

- Homework 1 released, due Thursday, Sept 26,11:55pm via Gradescope
  - Upload homework well in advance
  - Check late day policy

- Optional discussion section this Friday, Sept 13, 11-12am, CS 142
  - Python setup, Google collab, Basics of Python & Numpy
  - Schedule for the remaining discussion sections listed on the lectures page

- Change in Oindrila’s office hours, Fridays 9-11am, CS 207

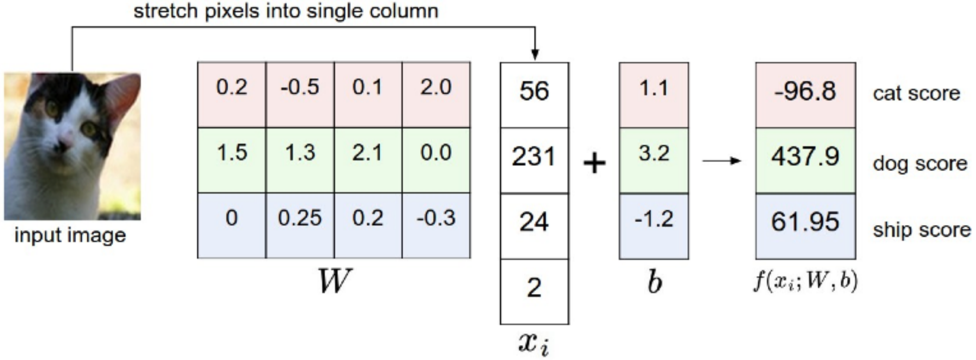
- Reminder to read course policies https://cvl-umass.github.io/compsci682-fall-2024/policies/ and course page in general

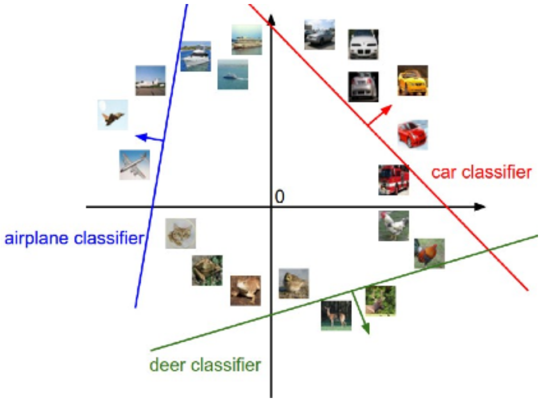
Recall from last time ... Linear classifier

[32x32x3]
array of numbers 0...1
(3072 numbers total)

image parameters
$f(\mathbf{x},\mathbf{W})$

10 numbers, indicating class scores





Loss function/Optimization



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

Goals:

- Define a **loss function** that quantifies our unhappiness with the scores across the training data.
- Come up with a way of efficiently finding the parameters that minimize the loss function. (**optimization**)

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**

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

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: $s_i = f(x_i, W)$

the SVM loss has the form:

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

and the full training loss is the mean over all examples in the training data:

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i$$

L = (2.9 + 0 + 12.9)/3
= **5.3**

Example numpy code:

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

```
def L_i_vectorized(x, y, W):
  scores = W.dot(x)
  margins = np.maximum(0, scores - scores[y] + 1)
  margins[y] = 0
  loss_i = np.sum(margins)
  return loss_i
```

Coding tip: Keep track of dimensions:

```
N = X.shape[0]
D = X.shape[1]
C = W.shape[1]

scores=X.dot(W)                 # (N,D)*(D,C)=(N,C)
```

Softmax Classifier (Multinomial Logistic Regression)

cat	**3.2**
car	5.1
frog	-1.7

Softmax Classifier (Multinomial Logistic Regression)

scores = unnormalized log probabilities of the classes.

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

cat	**3.2**
car	5.1
frog	-1.7

Softmax Classifier (Multinomial Logistic Regression)

scores = unnormalized log probabilities of the classes.

$$\boxed{P(Y=k|X=x_i)=\frac{e^{s_k}}{\sum_j e^{s_j}}}$$ where $$\boxed{s=f(x_i;W)}$$

cat	**3.2**
car	5.1
frog	-1.7

Softmax Classifier (Multinomial Logistic Regression)

scores = unnormalized log probabilities of the classes.

$$P(Y = k|X = x_i) = \boxed{\frac{e^{s_k}}{\sum_j e^{s_j}}} \quad \text{where} \quad s = f(x_i; W)$$

Softmax function

cat	**3.2**
car	5.1
frog	-1.7

Softmax Classifier (Multinomial Logistic Regression)

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scores = unnormalized log probabilities of the classes.

$$\boxed{P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}}$$ where $$\boxed{s = f(x_i; W)}$$

Want to maximize the log likelihood, or (for a loss function) to minimize the negative log likelihood of the correct class:

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

Softmax Classifier (Multinomial Logistic Regression)

cat	**3.2**
car	5.1
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scores = unnormalized log probabilities of the classes.

$$\boxed{P(Y=k|X=x_i)=\frac{e^{s_k}}{\sum_j e^{s_j}}}$$ where $$\boxed{s=f(x_i;W)}$$

Want to maximize the log likelihood, or (for a loss function) to minimize the negative log likelihood of the correct class:

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

---

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

Softmax Classifier (Multinomial Logistic Regression)

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

cat	**3.2**
car	5.1
frog	-1.7

unnormalized log probabilities

Softmax Classifier (Multinomial Logistic Regression)

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

unnormalized probabilities

cat	**3.2**	$\xrightarrow{\text{exp}}$	**24.5**
car	5.1		164.0
frog	-1.7		0.18

unnormalized log probabilities

Softmax Classifier (Multinomial Logistic Regression)

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

unnormalized probabilities

cat	**3.2**	**24.5**	**0.13**
car	5.1	164.0	0.87
frog	-1.7	0.18	0.00

$\xrightarrow{\text{exp}}$ $\xrightarrow{\text{normalize}}$

unnormalized log probabilities

probabilities
>0, sum to 1

Softmax Classifier (Multinomial Logistic Regression)

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

unnormalized probabilities

	unnormalized log probabilities	exp	unnormalized probabilities	normalize	probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

$\rightarrow$ L_i = -log(0.13)
= **0.89**

unnormalized log probabilities

probabilities

Softmax Classifier (Multinomial Logistic Regression)

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

unnormalized probabilities

	unnormalized log probabilities	exp →	unnormalized probabilities	normalize →	probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

→ L_i = -log(0.13)
= **0.89**

unnormalized log probabilities

probabilities

Softmax Classifier (Multinomial Logistic Regression)

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

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

unnormalized probabilities

	unnormalized log probabilities	exp →	unnormalized probabilities	normalize →	probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

→ L_i = -log(0.13)
= **0.89**

unnormalized log probabilities

probabilities

Softmax Classifier (Multinomial Logistic Regression)

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

Q2: usually at initialization W are small numbers, so all s ~= 0. What is the loss?

unnormalized probabilities

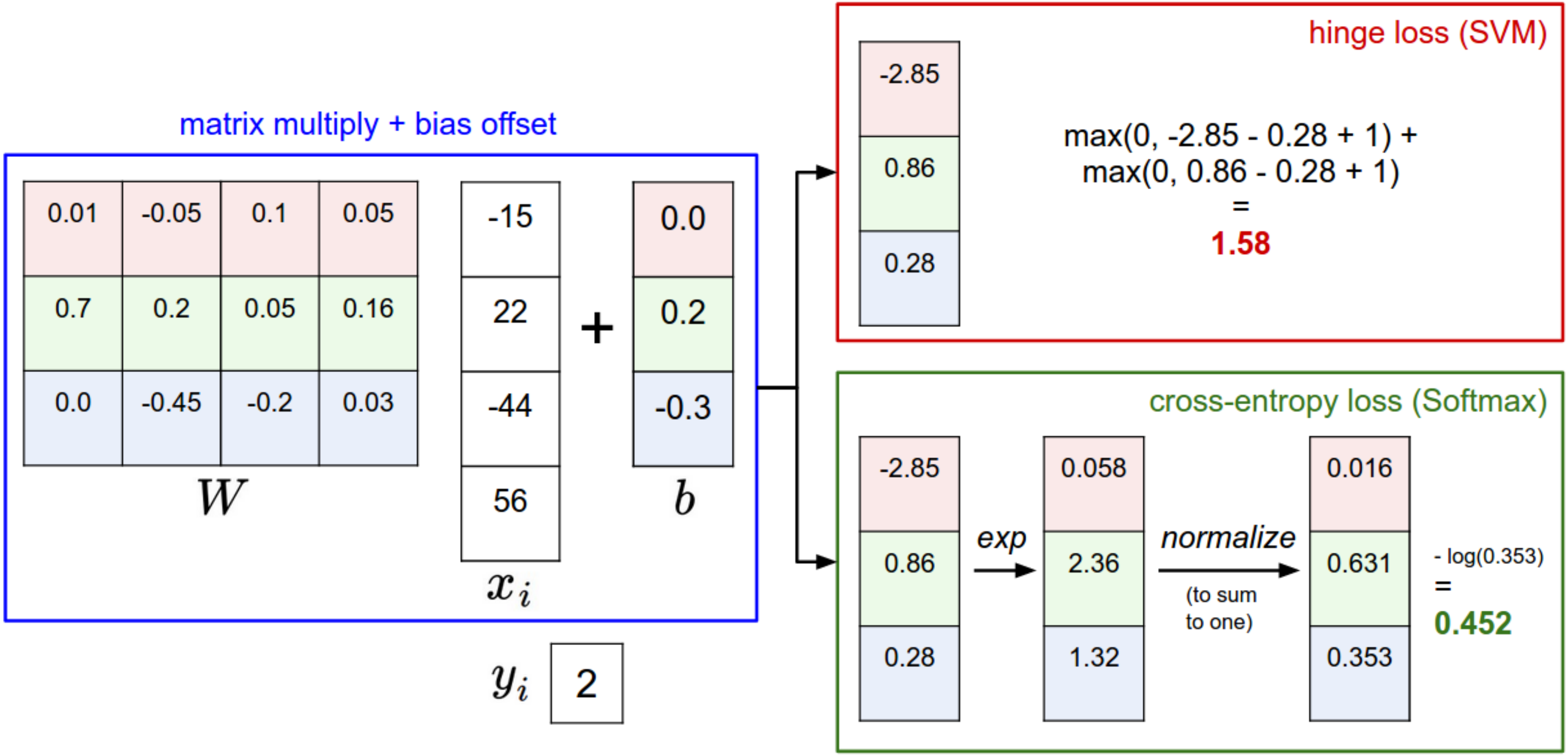
	unnormalized log probabilities	exp →	unnormalized probabilities	normalize →	probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

→ L_i = -log(0.13)
= **0.89**

Softmax vs. SVM

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

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


matrix multiply + bias offset
0.01
-0.05
0.1
0.05
0.7
0.2
0.05
0.16
0.0
-0.45
-0.2
0.03
W
-15
22
-44
56
x_i
+
0.0
0.2
-0.3
b
y_i
2
hinge loss (SVM)
-2.85
0.86
0.28
max(0, -2.85 - 0.28 + 1) +
max(0, 0.86 - 0.28 + 1)
=
1.58
cross-entropy loss (Softmax)
-2.85
0.86
0.28
exp
0.058
2.36
1.32
normalize
(to sum
to one)
0.016
0.631
0.353
- log(0.353)
=
0.452

Softmax vs. SVM

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

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

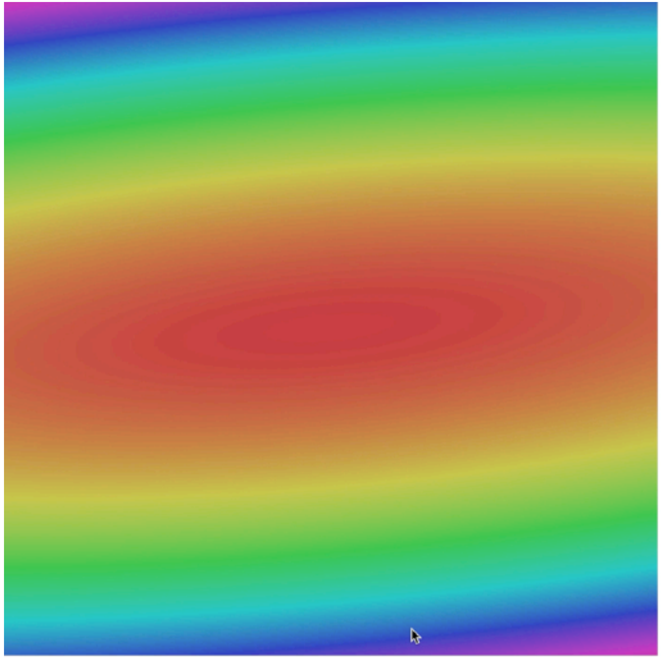
assume scores:
[10, -2, 3]
[10, 9, 9]
[10, -100, -100]
and $\boxed{y_i = 0}$

Q: Suppose I take a datapoint and I jiggle a bit (changing its score slightly). What happens to the loss in both cases?

Coming up:

- Regularization
- Optimization

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



Regularization

There is a "bug" with the loss:

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

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

E.g. Suppose that we found a W such that L = 0.
Is this W unique?

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

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car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	12.9

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

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

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

An example:

What is the loss? (POLL)

cat	1.3
car	**2.5**
frog	2.0

Loss:

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

An example:

What is the loss?

cat	1.3
car	**2.5**
frog	2.0
Loss:	0.5

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

cat	1.3
car	**2.5**
frog	2.0
Loss:	0.5

An example:
What is the loss?

How could we change W to eliminate the loss? (POLL)

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

cat	1.3	2.6
car	**2.5**	**5.0**
frog	2.0	4.0
Loss:	0.5	0

An example:
What is the loss?

How could we change W to eliminate the loss? (POLL)

Multiply W (and b) by 2!

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

cat	1.3	2.6
car	**2.5**	**5.0**
frog	2.0	4.0
Loss:	0.5	0

An example:
What is the loss?

How could we change W to eliminate the loss? (POLL)

Multiply W (and b) by 2!

Wait a minute! Have we done anything useful???

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

cat	1.3	2.6
car	**2.5**	**5.0**
frog	2.0	4.0
Loss:	0.5	0

An example:
What is the loss?

How could we change W to eliminate the loss? (POLL)

Multiply W (and b) by 2!

Wait a minute! Have we done anything useful???

No! Any example that used to be wrong is still wrong (on the wrong side of the boundary). Any example that is right is still right (on the correct side of the boundary).

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 having too much flexibility.

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:

Dropout

Batch normalization

Stochastic depth, fractional pooling, etc

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 having too much flexibility.

Why regularize?

- Express preferences over weights
- Make the model *simple* so it works on test data
- Improve optimization by adding curvature

Regularization: Expressing Preferences

$$x = [1, 1, 1, 1]$$

$$w_1 = [1, 0, 0, 0]$$

$$w_2 = [0.25, 0.25, 0.25, 0.25]$$

$$w_1^T x = w_2^T x = 1$$

L2 Regularization

$$R(W) = \sum_k \sum_l W_{k,l}^2$$

Regularization: Expressing Preferences

$$x = [1, 1, 1, 1]$$

$$w_1 = [1, 0, 0, 0]$$

$$w_2 = \boxed{[0.25, 0.25, 0.25, 0.25]}$$

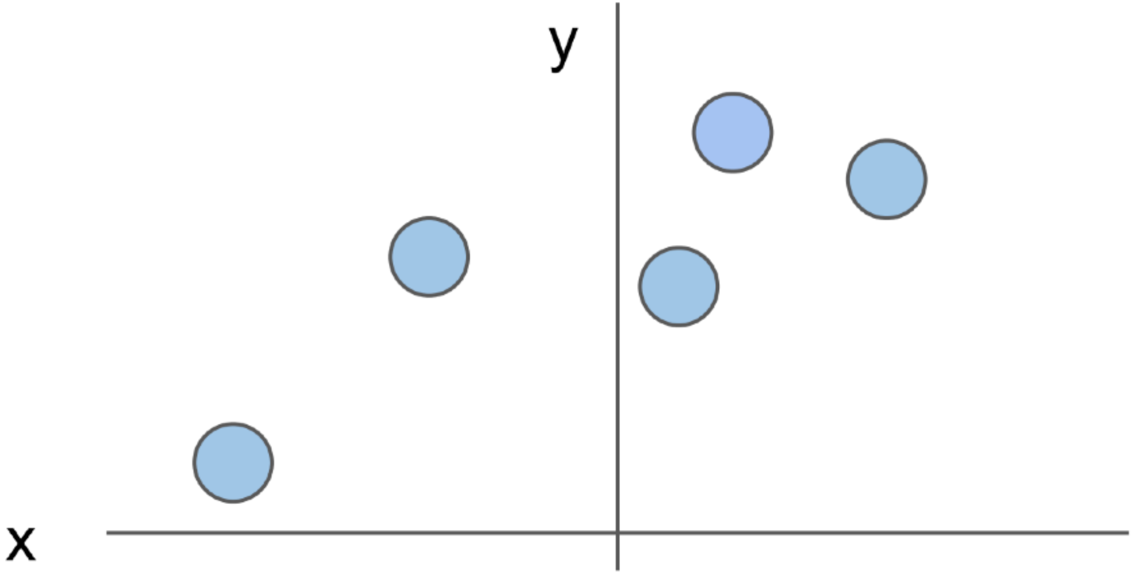
$$w_1^T x = w_2^T x = 1$$

L2 Regularization

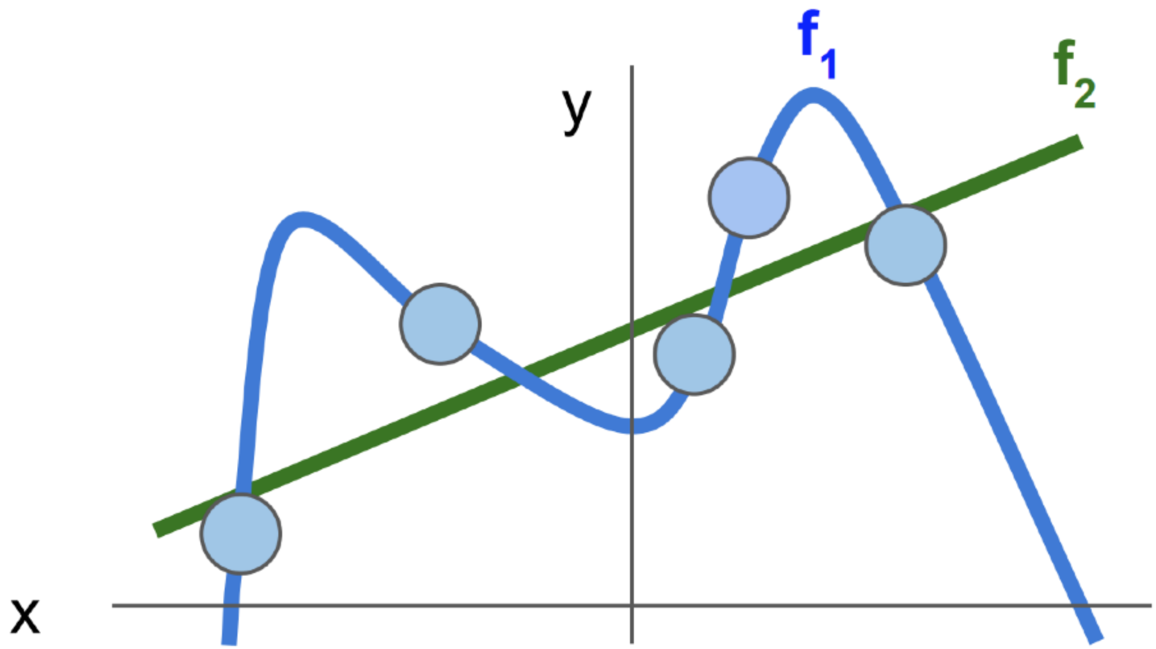
$$R(W) = \sum_k \sum_l W_{k,l}^2$$

L2 regularization likes to "spread out" the weights

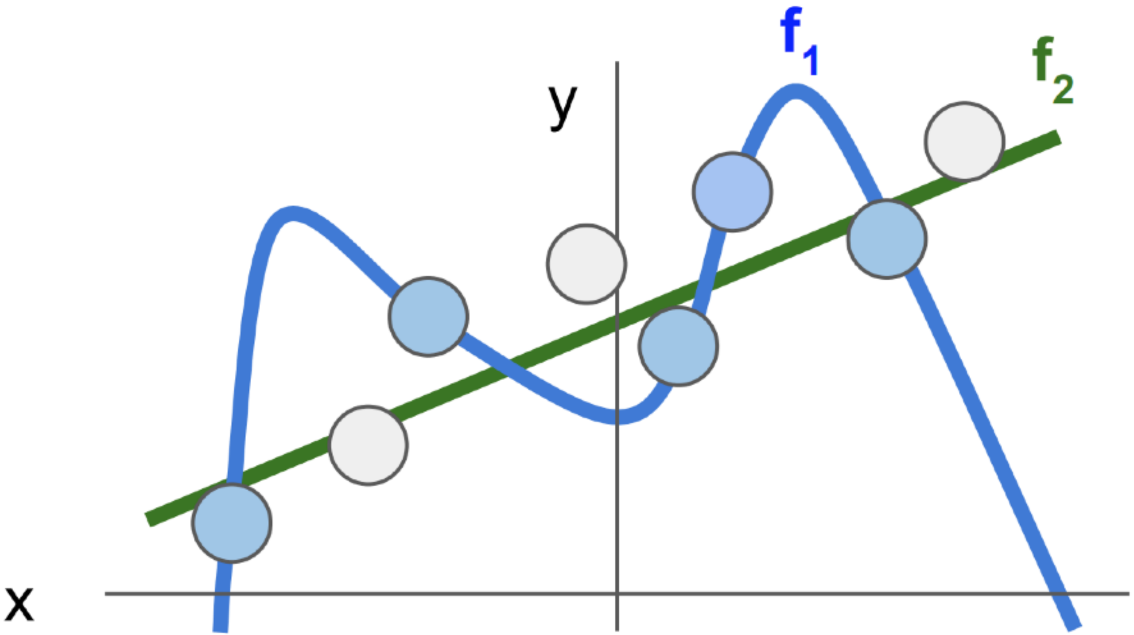
Regularization: Prefer Simpler Models



Regularization: Prefer Simpler Models



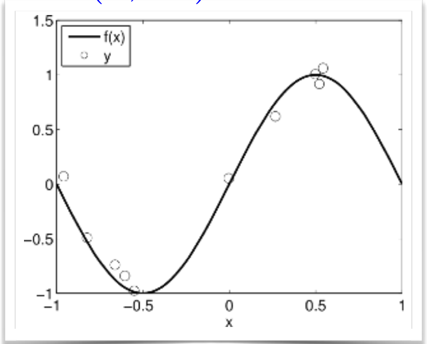
Regularization: Prefer Simpler Models



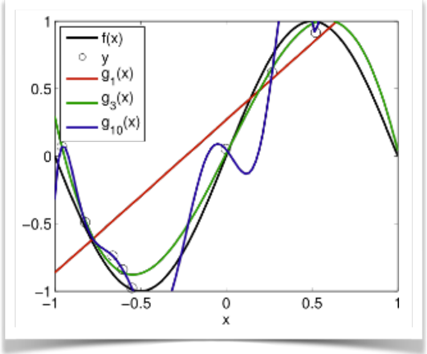
Regularization pushes against fitting the data with too much flexibility. If you are going to use a complex function to fit the data, you should be doing based on a lot of data!

Bias Variance Tradeoff

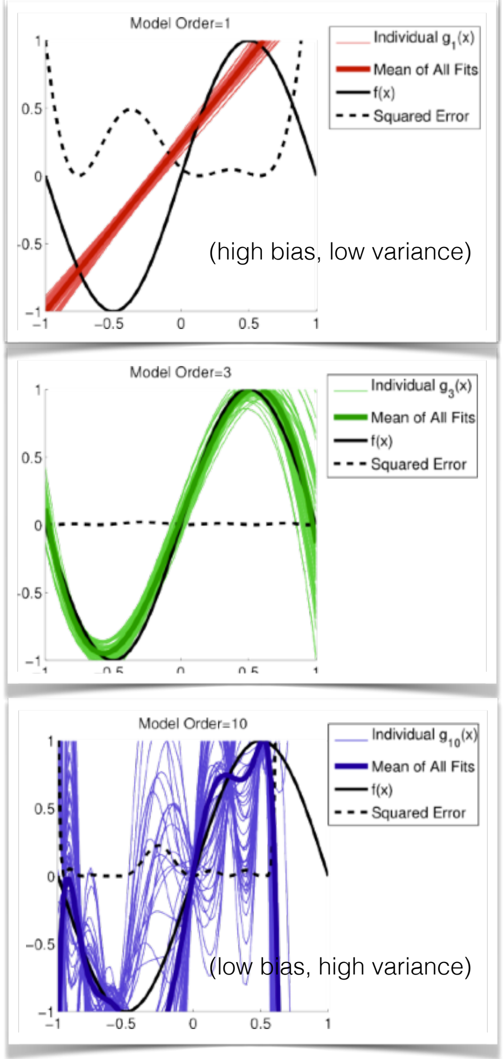
$$y = f(x) + \epsilon \quad f(x) = \sin(\pi x)$$
$$\epsilon = N(0, \sigma^2) \quad \sigma = 0.1$$



$$g_n(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_n x^n$$

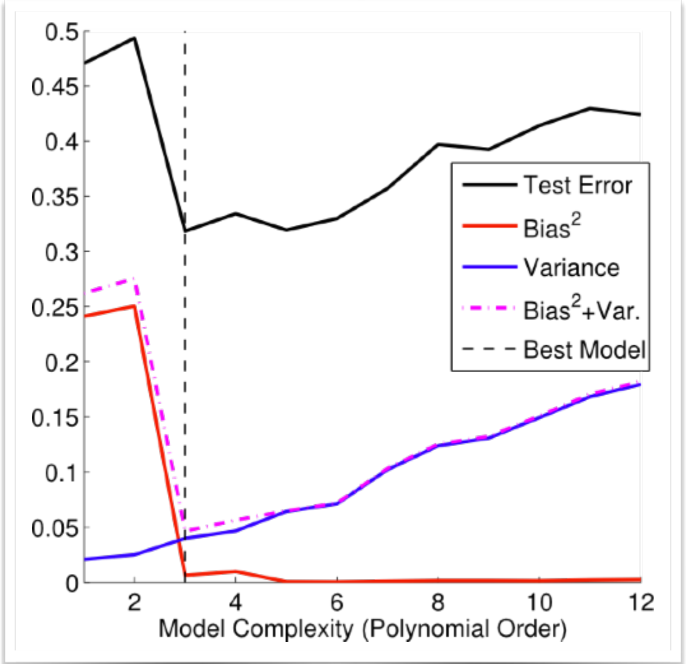


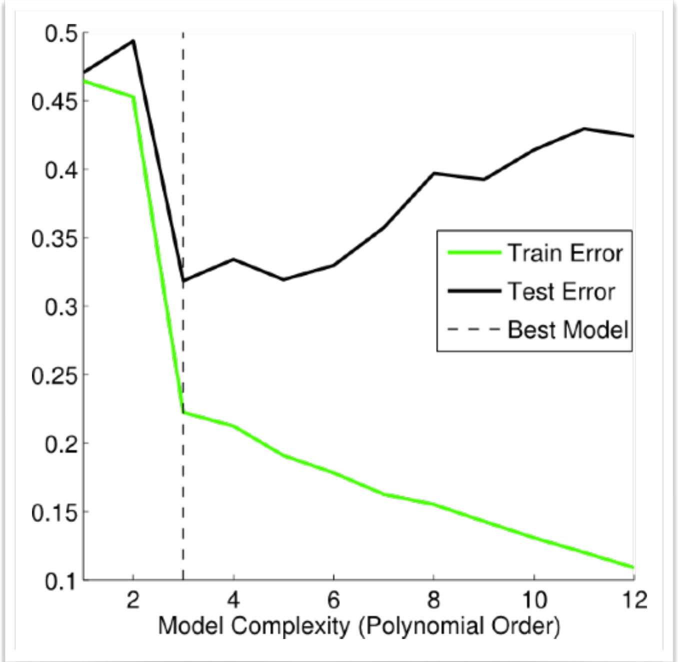
50 samples



figures from https://theclevermachine.wordpress.com/tag/estimator-variance/

Bias Variance Tradeoff for Polynomials

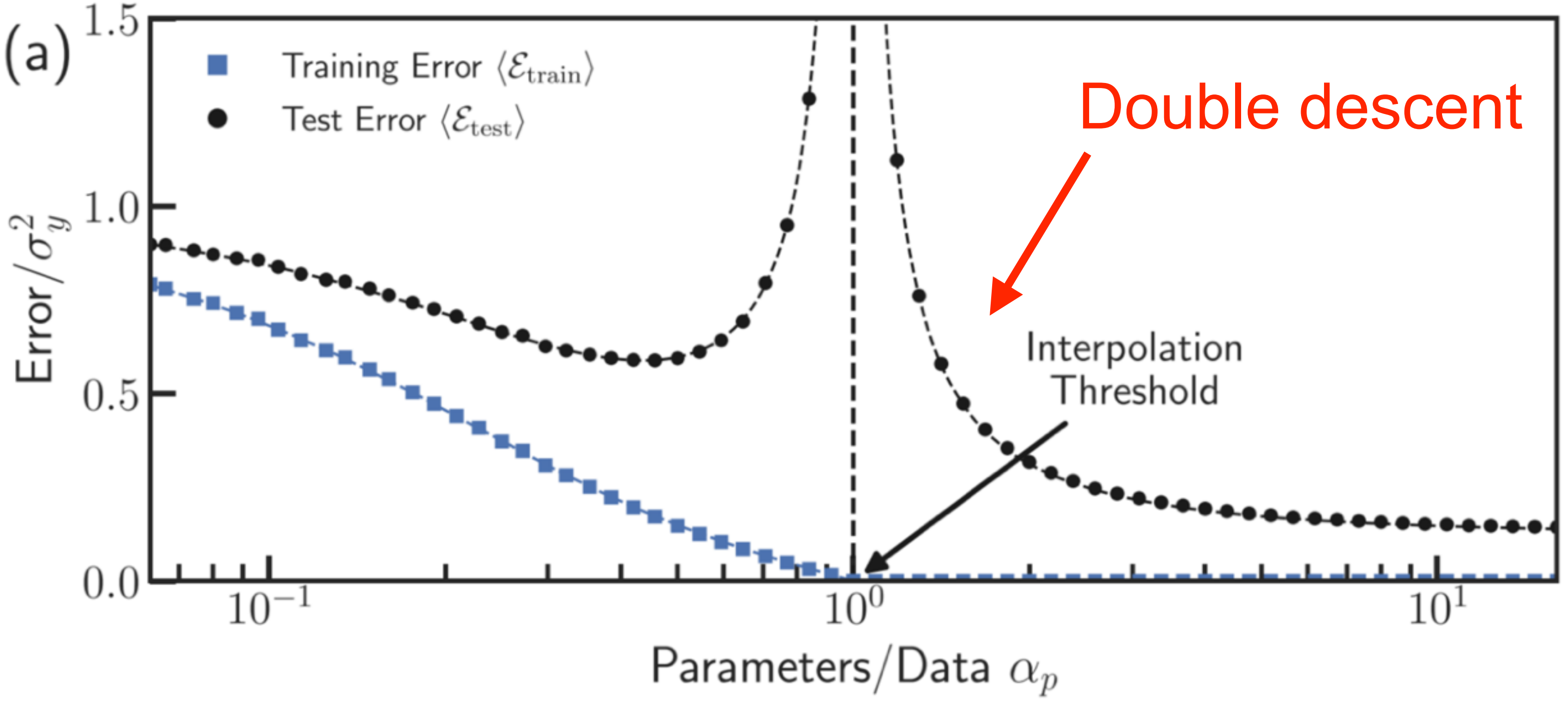




figures from https://theclevermachine.wordpress.com/tag/estimator-variance/

But things can be complicated!

Source: https://en.wikipedia.org/wiki/Double_descent



Optimization

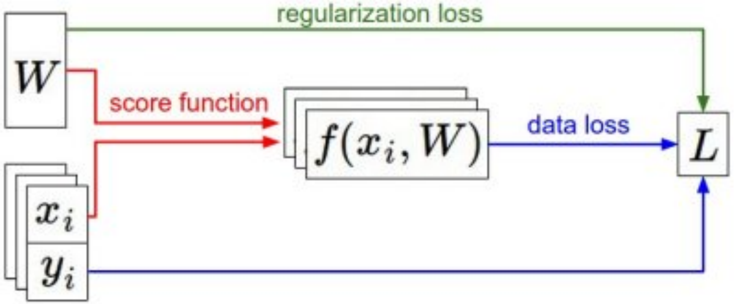
Recap

- We have some dataset of (x,y)
- We have a **score function:** $s = f(x; W) \overset{\text{e.g.}}{=} Wx$
- We have a **loss function**:

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

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

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + R(W)$$ Full loss



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

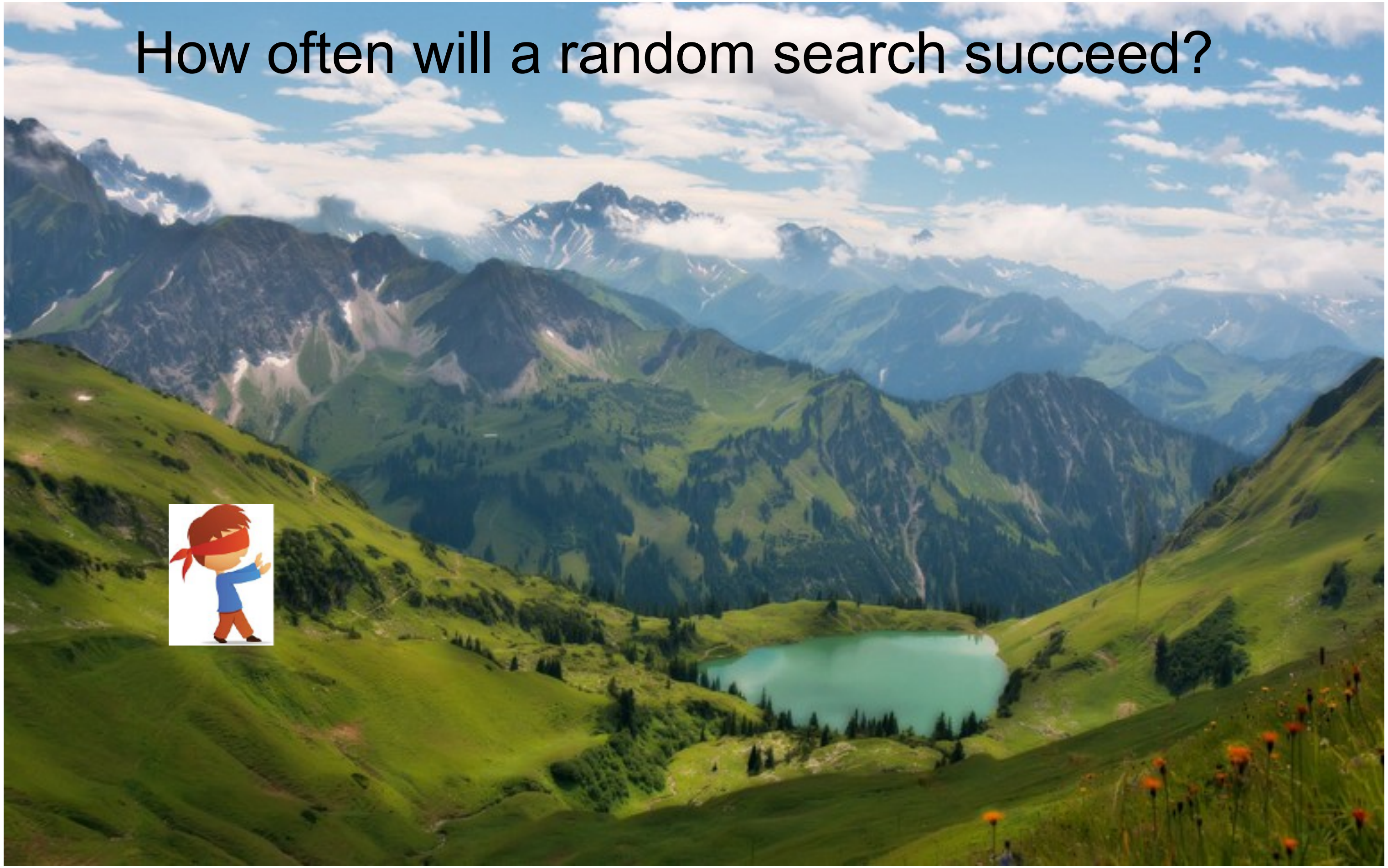
```
# assume X_train is the data where each column is an example (e.g. 3073 x 50,000)
# assume Y_train are the labels (e.g. 1D array of 50,000)
# assume the function L evaluates the loss function

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
# ... (truncated: continues for 1000 lines)
```

Let's see how well this works on the test set...

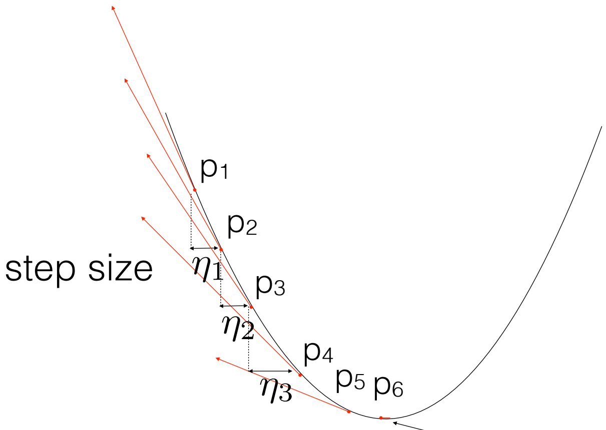
```
# Assume X_test is [3073 x 10000], Y_test [10000 x 1]
scores = Wbest.dot(Xte_cols) # 10 x 10000, the class scores for all test examples
# find the index with max score in each column (the predicted class)
Yte_predict = np.argmax(scores, axis = 0)
# and calculate accuracy (fraction of predictions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

15.5% accuracy! not bad!
(SOTA is ~95%)

How often will a random search succeed?



Strategy #2: **Follow the slope**



$$g^{(k)} \leftarrow \nabla_p F(p)|_{p_k}$$

compute gradient at the current location

$$p_{k+1} \leftarrow p_k - \eta_k g^{(k)}$$

take a step down the gradient

local optima = global optima

Strategy #2: **Follow the slope**

In 1-dimension, the derivative of a function:

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

In multiple dimensions, the **gradient** is the vector of (partial derivatives).

A sneak "preview" of the motivation for backpropagation

Consider the function

$$z(x, y) = x^2 + y^2,$$

and suppose we are interested in evaluating the gradient of this function at the point

$$(x, y) = (5, 3).$$

Evaluate the gradient:

$$\frac{\partial z}{\partial x} = 2x.$$

$$\frac{\partial z}{\partial y} = 2y.$$

The algebraic expression of the gradient is just the collection of these partials into a "vector":

$$\nabla z = \begin{bmatrix} 2x \\ 2y \end{bmatrix}.$$

Don't care about this

The evaluation of this gradient at the point $(x, y) = (5, 3)$ is simply

$$\nabla z(5, 3) = \begin{bmatrix} 2 \times 5 \\ 2 \times 3 \end{bmatrix} = \begin{bmatrix} 10 \\ 6 \end{bmatrix}.$$

Do care about this

Numerical evaluation of the gradient...

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:

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

W + h (first dim)**:**

[0.34 + **0.0001**,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25322

gradient dW:

[?,
?,
?,
?,
?,
?,
?,
?,
?,…]

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

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

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,
?,
?,
?,
?,
?,
?,
?,
?,…]

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

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

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

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

current W:

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

dW = ...
(some function of
data and W)

gradient dW:

[-2.5,
0.6,
0,
0.2,
0.7,
-0.5,
1.1,
1.3,
-2.1,…]

Evaluating the gradient numerically

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

```python
def eval_numerical_gradient(f, x):
  """
  a naive implementation of numerical gradient of f at x
  - f should be a function that takes a single argument
  - x is the point (numpy array) to evaluate the gradient at
  """

  fx = f(x) # evaluate function value at original point
  grad = np.zeros(x.shape)
  h = 0.00001

  # iterate over all indexes in x
  it = np.nditer(x, flags=['multi_index'], op_flags=['readwrite'])
  while not it.finished:

    # evaluate function at x+h
    ix = it.multi_index
    old_value = x[ix]
    x[ix] = old_value + h # increment by h
    fxh = f(x) # evalute f(x + h)
    x[ix] = old_value # restore to previous value (very important!)

    # compute the partial derivative
    grad[ix] = (fxh - fx) / h # the slope
    it.iternext() # step to next dimension

  return grad
```

Evaluating the gradient numerically

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

- approximate
- very slow to evaluate

```python
def eval_numerical_gradient(f, x):
  """
  a naive implementation of numerical gradient of f at x
  - f should be a function that takes a single argument
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  while not it.finished:

    # evaluate function at x+h
    ix = it.multi_index
    old_value = x[ix]
    x[ix] = old_value + h # increment by h
    fxh = f(x) # evalute f(x + h)
    x[ix] = old_value # restore to previous value (very important!)

    # compute the partial derivative
    grad[ix] = (fxh - fx) / h # the slope
    it.iternext() # step to next dimension

  return grad
```