English for Computer Science

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Lecture5:
Optimization

Summary

- We defined a **score function** from image pixels to class scores (in this section, a linear function that depends on weights **W** and biases **b**).
- Unlike kNN classifier, the advantage of this **parametric approach** is that once we learn the parameters we can discard the training data. Additionally, the prediction for a new test image is fast since it requires a single matrix multiplication with **W**, not an exhaustive comparison to every single training example.
- We defined a **loss function** (we introduced two commonly used losses for linear classifiers: the **SVM** and the **Softmax**) that measures how compatible a given set of parameters is with respect to the ground truth labels in the training dataset. We also saw that the loss function was defined in such way that making good predictions on the training data is equivalent to having a small loss.

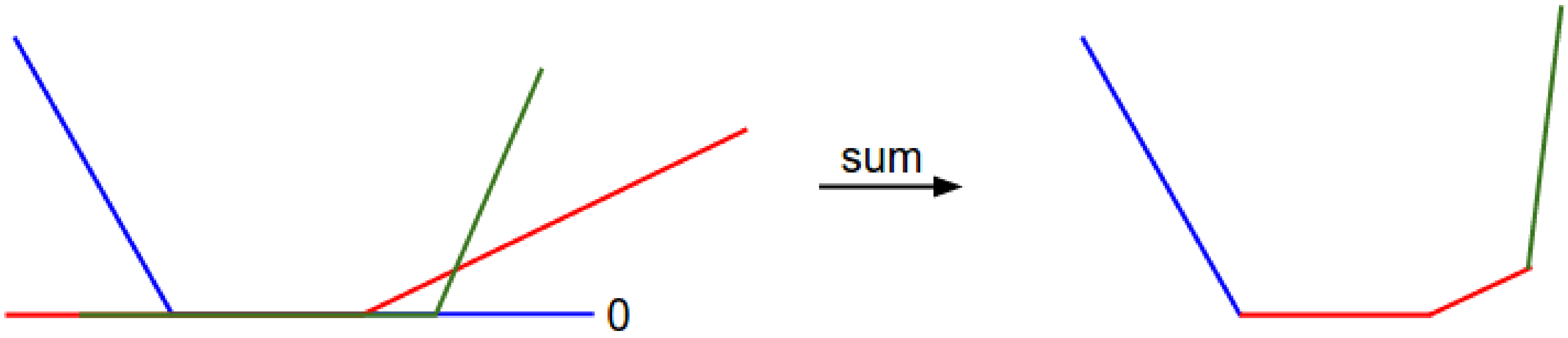
Visualizing the loss function

$$L_0 = \max(0, w_1^T x_0 - w_0^T x_0 + 1) + \max(0, w_2^T x_0 - w_0^T x_0 + 1)$$

$$L_1 = \max(0, w_0^T x_1 - w_1^T x_1 + 1) + \max(0, w_2^T x_1 - w_1^T x_1 + 1)$$

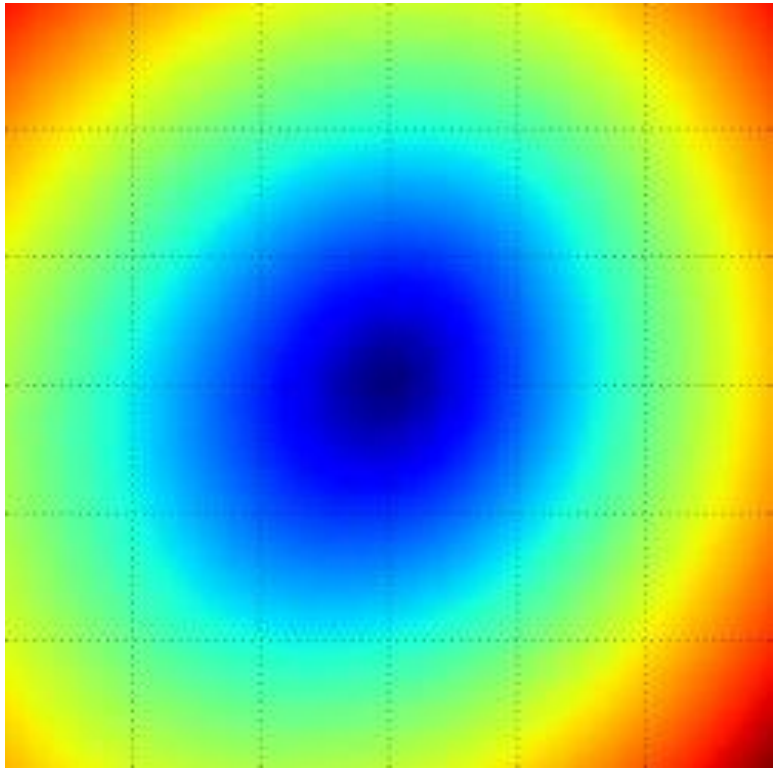
$$L_2 = \max(0, w_0^T x_2 - w_2^T x_2 + 1) + \max(0, w_1^T x_2 - w_2^T x_2 + 1)$$

$$L = (L_0 + L_1 + L_2)/3$$



Visualizing the loss function

Left: one-dimensional loss



Right: two-dimensional loss slice, Blue = low loss, Red = high 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
# ... (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 ~95%)

Core idea: iterative refinement

- Of course, it turns out that we can do much better. The core idea is that finding the best set of weights **W** is a very difficult or even impossible problem (especially once **W** contains weights for entire complex neural networks).
- But the problem of refining a specific set of weights **W** to be slightly better is significantly less difficult.
- In other words, our approach will be to start with a random **W** and then iteratively refine it, making it slightly better each time.

Random Local Search

We will start out with a random W, generate a random value α, such that **W <- W+αW**, if the loss decreases, we will perform an update.

```
W = np.random.randn(10, 3073) * 0.001 # generate random starting W
bestloss = float("inf")
for i in xrange(1000):
  step_size = 0.0001
  Wtry = W + np.random.randn(10, 3073) * step_size
  loss = L(Xtr_cols, Ytr, Wtry)
  if loss < bestloss:
    W = Wtry
    bestloss = loss
  print 'iter %d loss is %f' % (i, bestloss)
```

This approach achieves test set classification accuracy of **21.4%**, better than the random (global) search (15.5%).

Strategy #2: **Follow the slope**

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) along each dimension

The slope in any direction is the **dot product** of the direction with the gradient
The direction of steepest descent is the **negative 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:

[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:

[**-2.5**,
?,
?,

(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:	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:

[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

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

?,…]

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

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,
?,
?,…]

Numeric Gradient

- Slow! Need to loop over all dimensions
- Approximate

This is silly. The loss is just a function of W:

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \sum_k W_k^2$$

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

$$s = f(x; W) = Wx$$

want $\nabla_W L$

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$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \sum_k W_k^2$$

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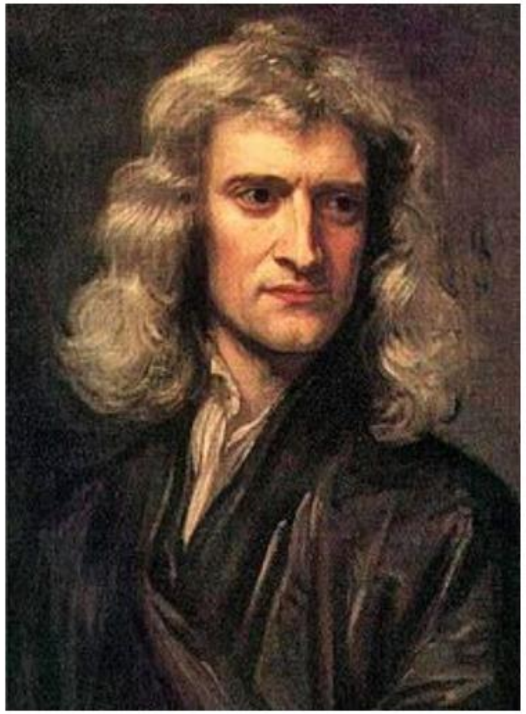
$$s = f(x; W) = Wx$$

want $\nabla_W L$



Use calculus to compute an **analytic gradient**

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
data and W)

gradient dW:

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

Analytical versus Numerical Approaches

Question: Find the root of $f(x)=x-5$.

Analytical solution:
$f(x)=x-5=0$, add +5 to both sides to get the answer $x=5$.

Numerical solution:
Let's guess $x=1$: $f(1)=1-5=-4$, A *negative* number.
Let's guess $x=6$: $f(6)=6-5=1$, A *positive* number.
The answer must be between them.
Let's try $x=(6+1)/2$: $f(7/2)<0$. So it must be between 7/2 and 6, repeat all above until $f(x)\approx x-5$.

Computing the gradient analytically with Calculus

- The **numerical gradient** is very simple to compute using the finite difference approximation, but the downside is that it is approximate (since we have to pick a small value of *h*, while the true gradient is defined as the limit as *h*->0), and that it is very computationally expensive to compute.
- The second way to compute the gradient is **analytically** using **Calculus**, which allows us to derive a direct formula for the gradient (no approximations) that is also very fast to compute. However, unlike the numerical gradient it can be more error prone to implement, which is why in practice it is very common to compute the analytic gradient and compare it to the numerical gradient to check the correctness of your implementation. This is called a **gradient check**.

Computing the gradient analytically with Calculus

Lets use the example of the SVM loss function for a single datapoint:

$$L_i = \sum_{j \neq y_i} \left[\max(0, w_j^T x_i - w_{y_i}^T x_i + \Delta) \right]$$

We can differentiate the function with respect to the weights. For example, taking the gradient with respect to w_{y_i} we obtain. Notice that this is the gradient only with respect to the row of W that corresponds to the correct class.

$$\nabla_{w_{y_i}} L_i = - \left(\sum_{j \neq y_i} \mathbb{1}(w_j^T x_i - w_{y_i}^T x_i + \Delta > 0) \right) x_i$$

For the other rows where $j \neq y_i$ the gradient is:

$$\nabla_{w_j} L_i = \mathbb{1}(w_j^T x_i - w_{y_i}^T x_i + \Delta > 0) x_i$$

In summary:

- Numerical gradient: approximate, slow, easy to write
- Analytic gradient: exact, fast, error-prone

=>

In practice: Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient check.**

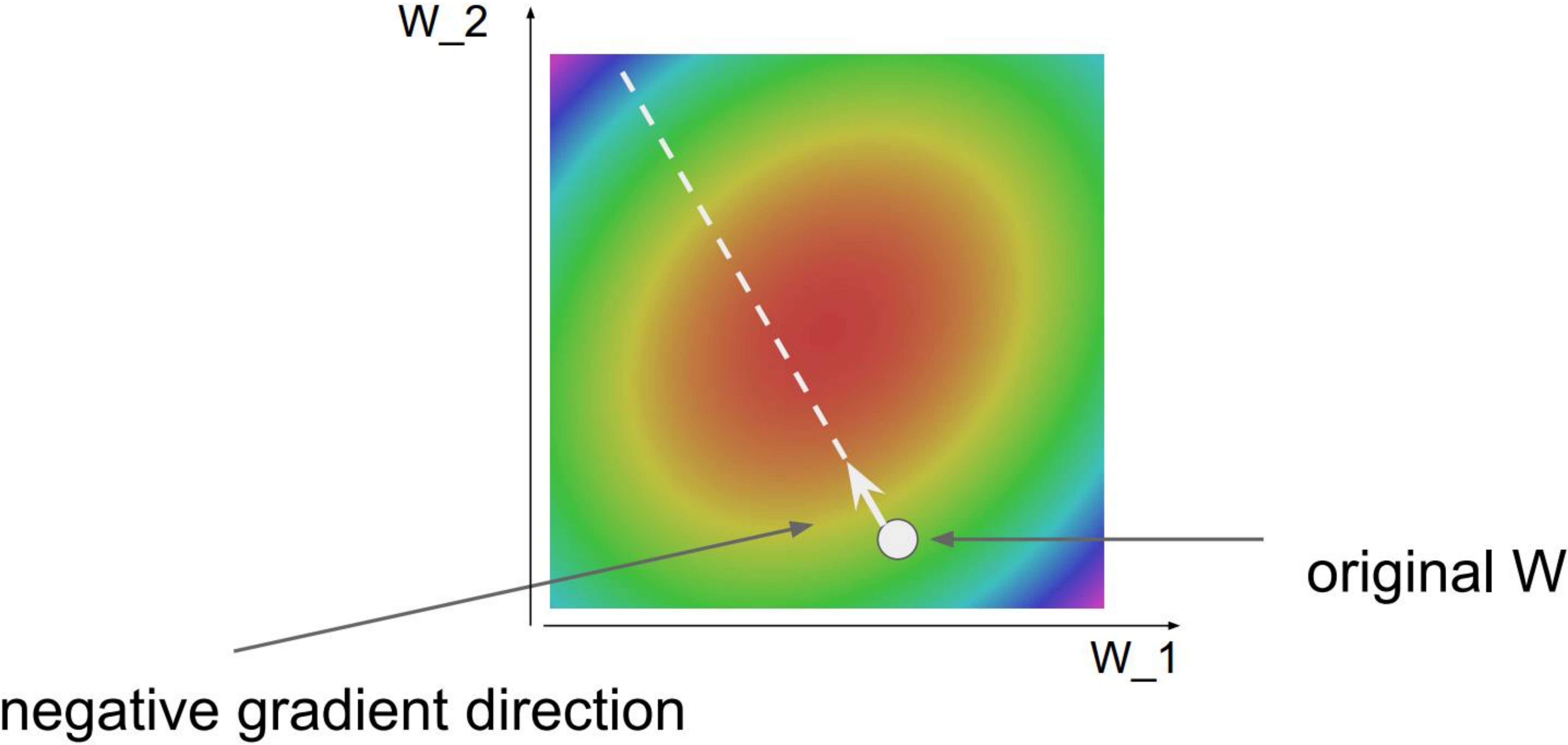
Gradient Descent

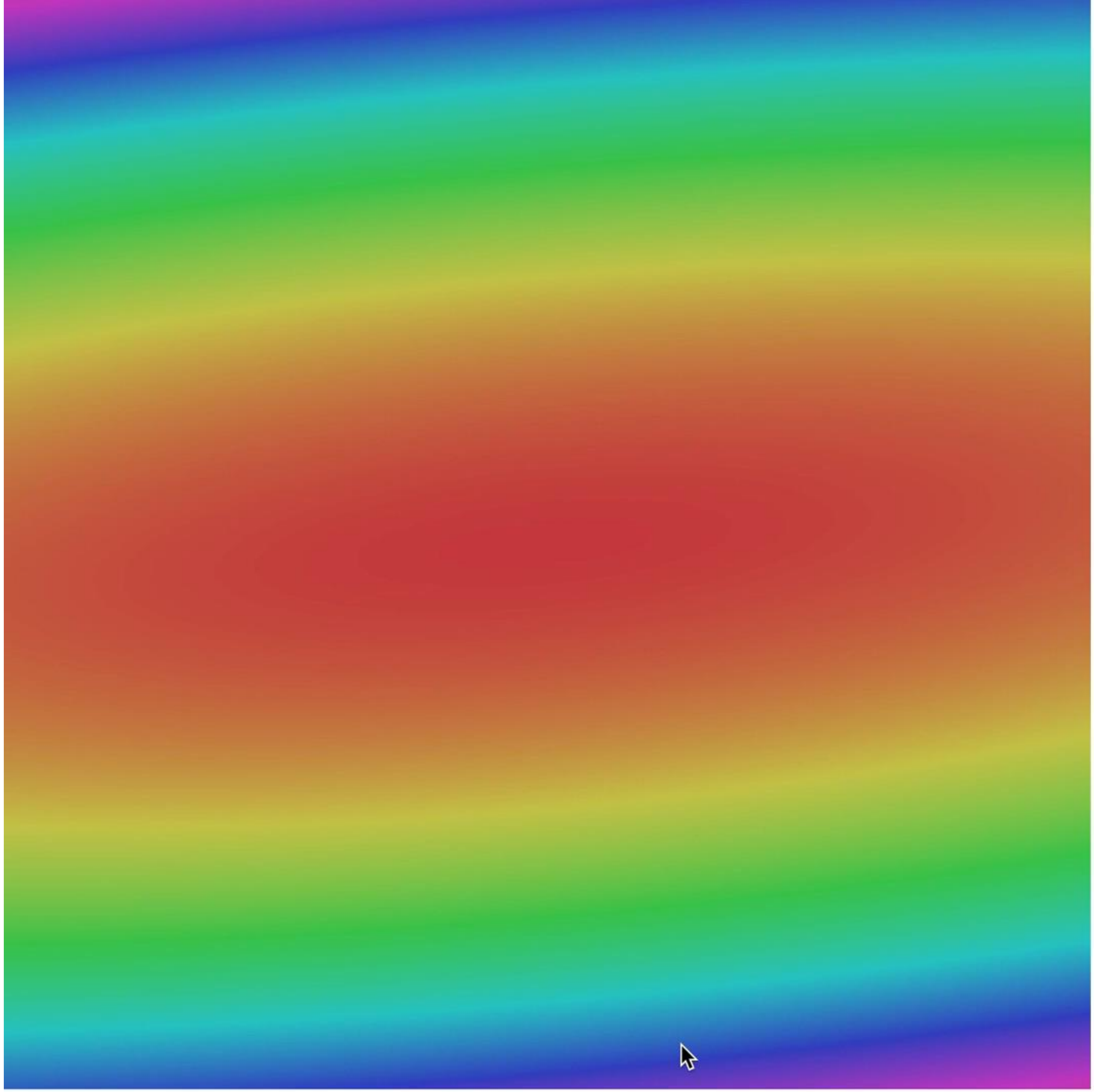
```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```

Update in negative gradient direction. In the code above, notice that to compute new weight, we are making an update in the negative direction of the gradient since we wish our loss function to decrease, not increase.

Visualizing the Gradient Descent





Mini-batch Gradient Descent

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

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

Full sum expensive when N is large!

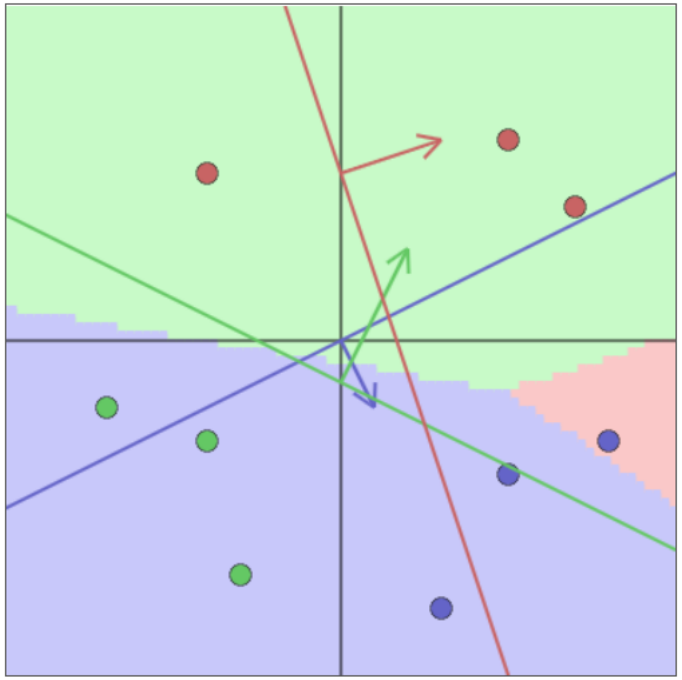
Approximate sum using a **minibatch** of examples
32 / 64 / 128 common

```
# Vanilla Minibatch Gradient Descent

while True:
  data_batch = sample_training_data(data, 256) # sample 256 examples
  weights_grad = evaluate_gradient(loss_fun, data_batch, weights)
  weights += - step_size * weights_grad # perform parameter update
```

Interactive web demo http://vision.stanford.edu/teaching/cs231n-demos/linear-classify/

Datapoints are shown as circles colored by their class (red/gree/blue). The background regions are colored by whichever class is most likely at any point according to the current weights. Each classifier is visualized by a line that indicates its zero score level set. For example, the blue classifier computes scores as $W_{0,0}x_0 + W_{0,1}x_1 + b_0$ and the blue line shows the set of points (x_0, x_1) that give score of zero. The blue arrow draws the vector $(W_{0,0}, W_{0,1})$, which shows the direction of score increase and its length is proportional to how steep the increase is.
Note: you can drag the datapoints.



Parameters W, b are shown below. The value is in **bold** and its gradient (computed with backprop) is in *red, italic* below. Click the triangles to control the parameters.

W[0,0]	W[0,1]	b[0]
▲	▲	▲
1.00 *-0.38*	**2.00** *0.07*	**0.00** *0.11*
▼	▼	▼
W[1,0]	W[1,1]	b[1]
▲	▲	▲
2.00 *0.51*	**-4.00** *-0.58*	**0.50** *-0.11*
▼	▼	▼
W[2,0]	W[2,1]	b[2]
▲	▲	▲
3.00 *0.17*	**-1.00** *0.36*	**-0.50** *0.00*
▼	▼	▼

Step size: 0.10000

Single parameter update

Start repeated update

Stop repeated update

Randomize parameters

Visualization of the data loss computation. Each row is loss due to one datapoint. The first three columns are the 2D data x_i and the label y_i. The next three columns are the three class scores from each classifier $f(x_i; W, b) = Wx_i + b$ (E.g. s[0] = x[0] * W[0,0] + x[1] * W[0,1] + b[0]). The last column is the data loss for a single example, L_i.

x[0]	x[1]	y	s[0]	s[1]	s[2]	L
0.50	0.40	0	1.30	-0.10	0.60	0.30
0.80	0.30	0	1.40	0.90	1.60	1.70
0.30	0.80	0	1.90	-2.10	-0.40	0.00
-0.40	0.30	1	0.20	-1.50	-2.00	3.20
-0.30	0.70	1	1.10	-2.90	-2.10	6.80
-0.70	0.20	1	-0.30	-1.70	-2.80	2.40
0.70	-0.40	2	-0.10	3.50	2.00	2.50
0.50	-0.60	2	-0.70	3.90	1.60	3.30
-0.40	-0.50	2	-1.40	1.70	-1.20	4.70
						mean:
						2.77

```
Total data loss: 2.77
Regularization loss: 3.50
Total loss: 6.27
```

L2 Regularization strength: 0.10000

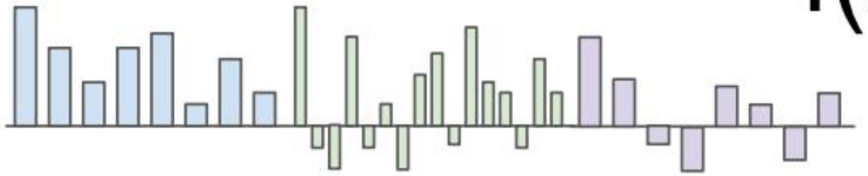
Multiclass SVM loss formulation:
- (●) Weston Watkins 1999
- ( ) One vs. All
- ( ) Structured SVM
- ( ) Softmax

Aside: Image Features

Class scores

$$f(x) = Wx$$

Aside: Image Features

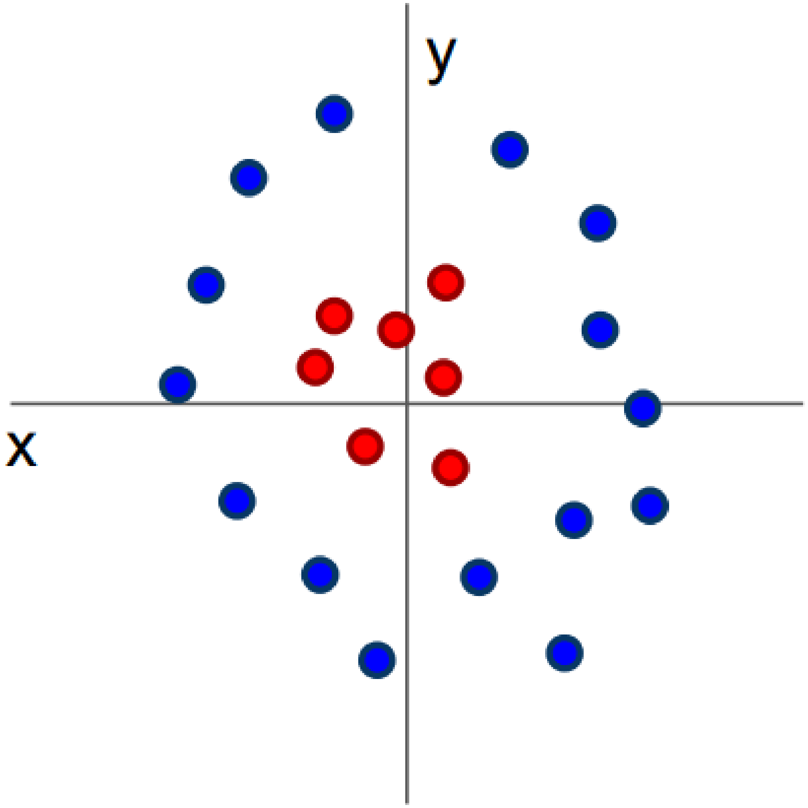


Feature Representation

$$f(x) = Wx$$

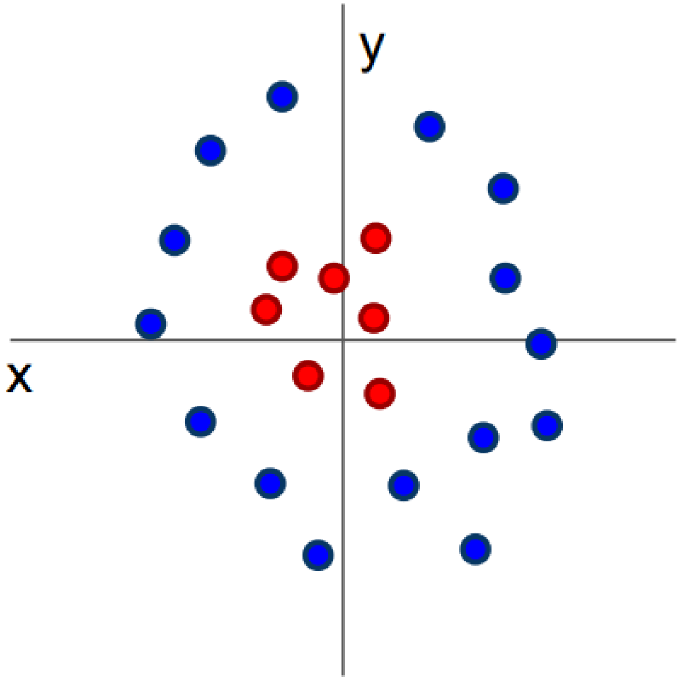
Class scores

Image Features: Motivation

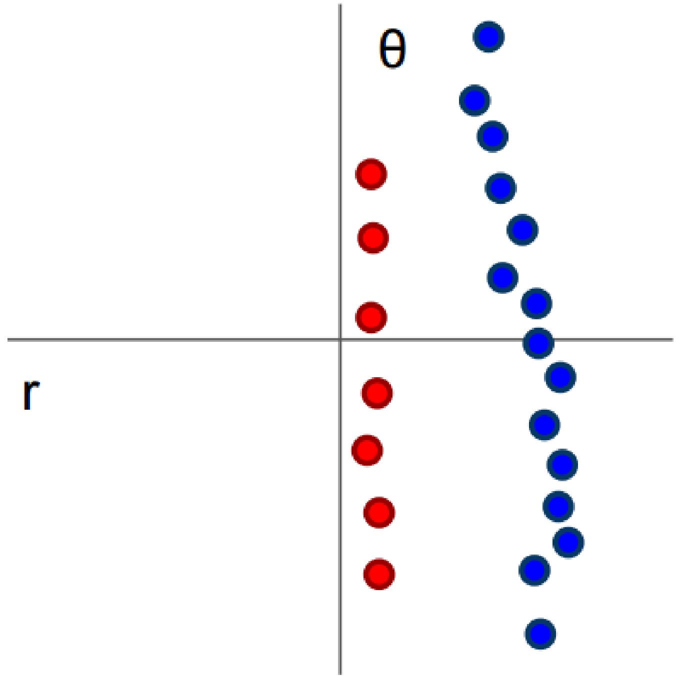


Cannot separate red and blue points with linear classifier

Image Features: Motivation



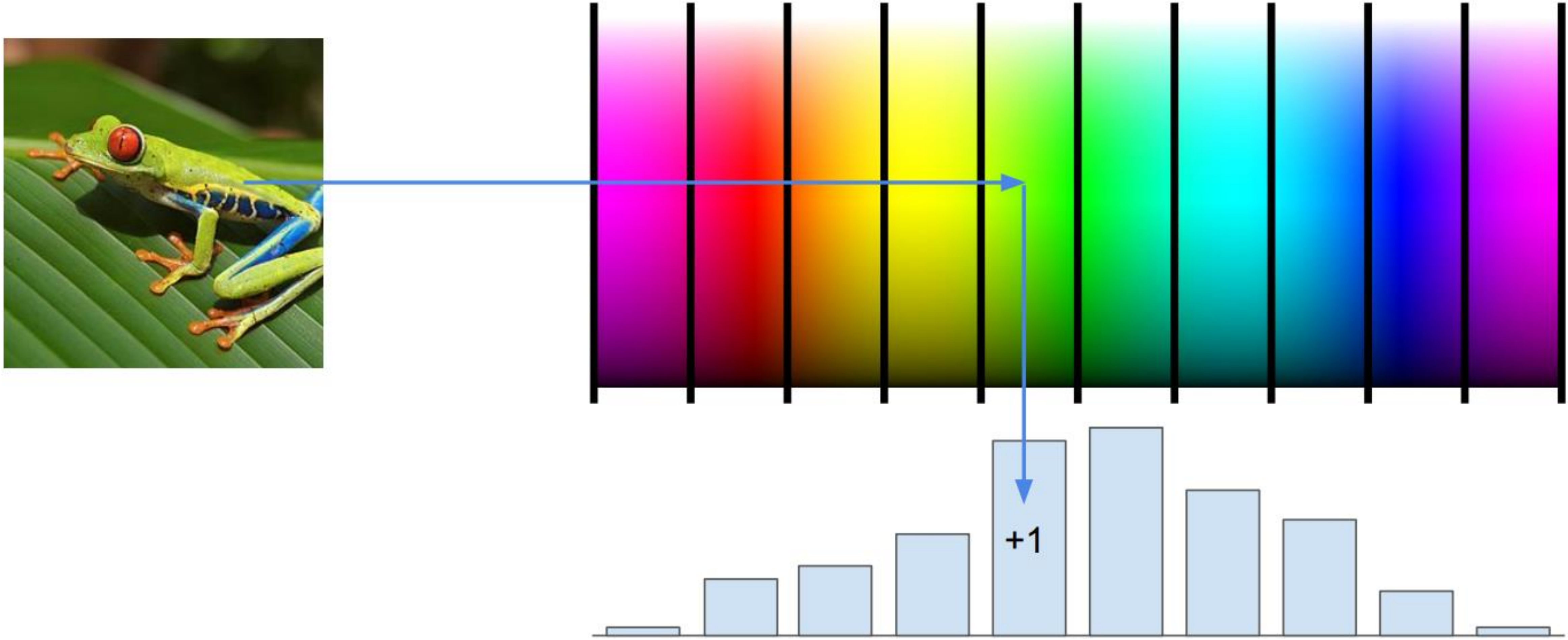
$$f(x, y) = (r(x, y), \theta(x, y))$$



Cannot separate red and blue points with linear classifier

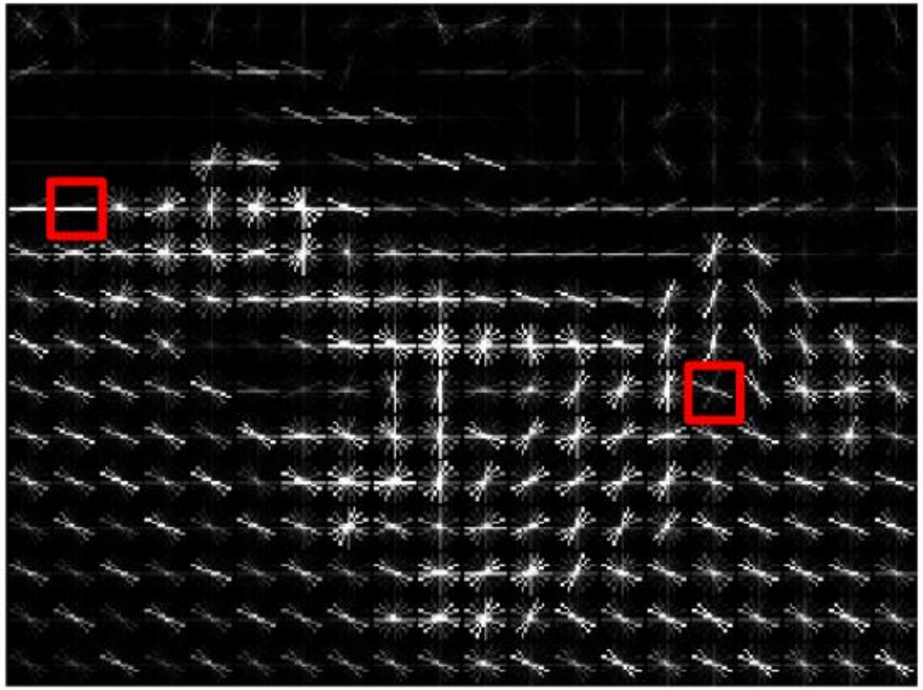
After applying feature transform, points can be separated by linear classifier

Example: Color Histogram



Example: Histogram of Oriented Gradients (HoG)

Divide image into 8x8 pixel regions
Within each region quantize edge direction into 9 bins



Example: 320x240 image gets divided into 40x30 bins; in each bin there are 9 numbers so feature vector has 30*40*9 = 10,800 numbers

Aside: Image Features

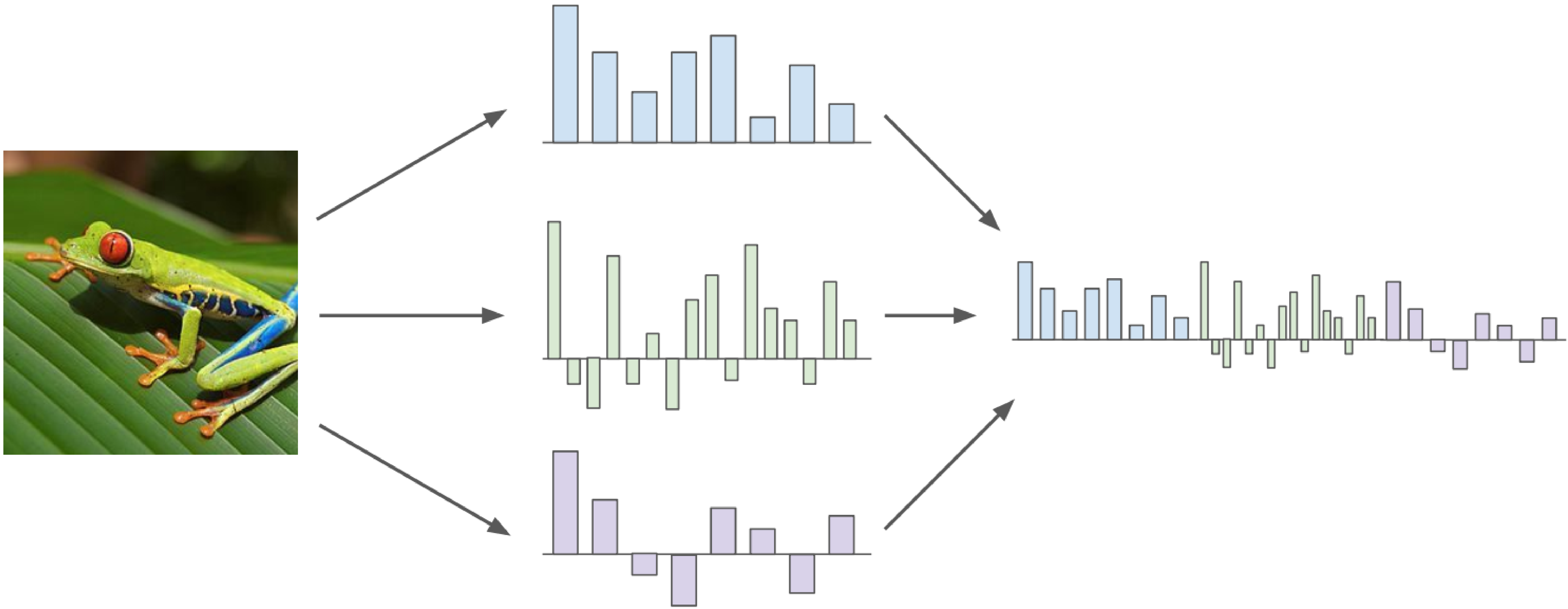


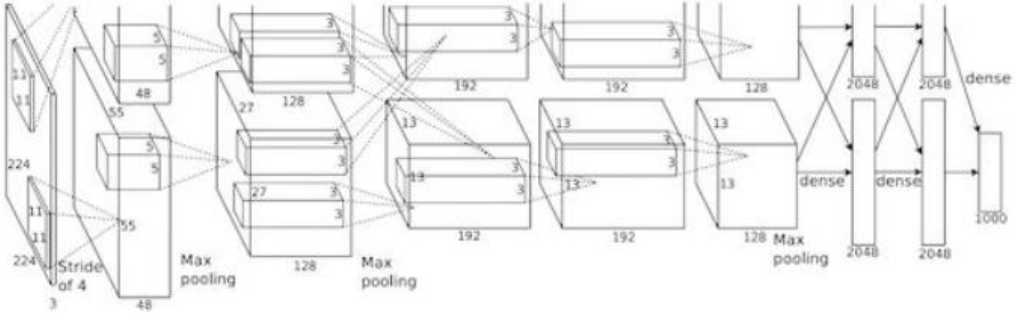
Image features vs ConvNets

Feature Extraction

f

10 numbers giving scores for classes

training



Krizhevsky, Sutskever, and Hinton, "Imagenet classification with deep convolutional neural networks", NIPS 2012.

10 numbers giving scores for classes

training

Next time:

Introduction to neural networks

Backpropagation