Lecture 2. First Approaches for Image Classification

Disclaimer: This note was modified from cs231n lecture notes by Prof. Li Fei-Fei at Stanford University.

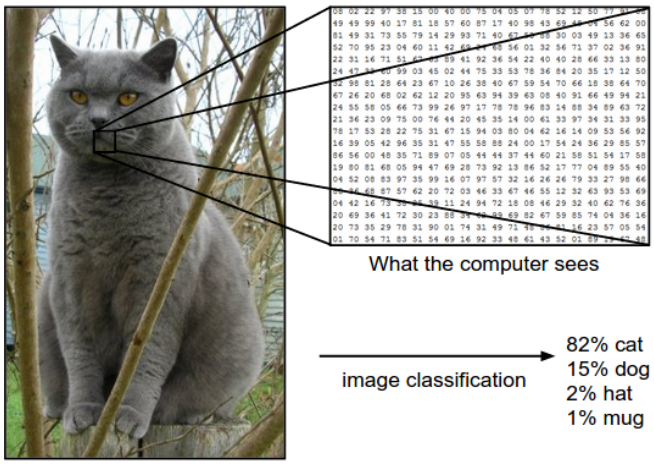
This is an introductory lecture designed to introduce people from outside of Computer Vision to the Image Classification problem, and the data-driven approach.

The Table of Contents:

Image Classification Task

Motivation. In this section we will introduce the Image Classification problem, which is the task of assigning an input image one label from a fixed set of categories. This is one of the core problems in Computer Vision that, despite its simplicity, has a large variety of practical applications. Moreover, as we will see later in the course, many other seemingly distinct Computer Vision tasks (such as object detection, segmentation) can be reduced to image classification.

Example. For example, in the image below an image classification model takes a single image and assigns probabilities to 4 labels, *{cat, dog, hat, mug}*. As shown in the image, keep in mind that to a computer an image is represented as one large 3-dimensional array of numbers. In this example, the cat image is 248 pixels wide, 400 pixels tall, and has three color channels Red,Green,Blue (or RGB for short). Therefore, the image consists of 248 x 400 x 3 numbers, or a total of 297,600 numbers. Each number is an integer that ranges from 0 (black) to 255 (white). Our task is to turn this quarter of a million numbers into a single label, such as *"cat"*.

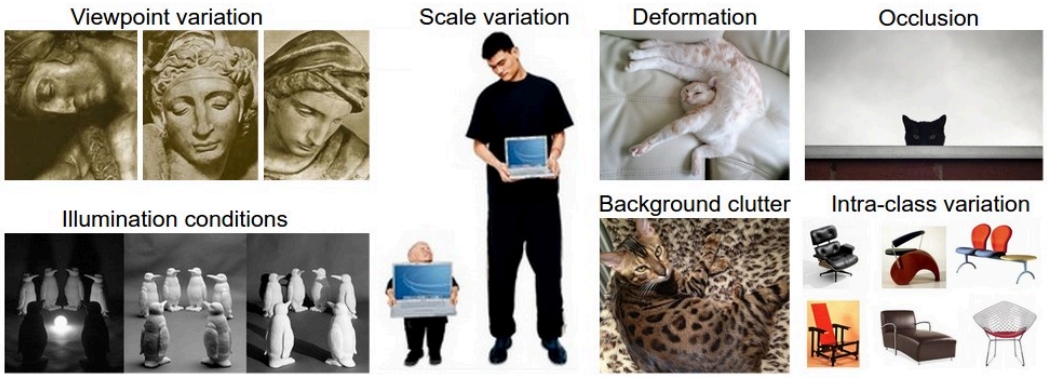


The task in Image Classification is to predict a single label (or a distribution over labels as shown here to indicate our confidence) for a given image. Images are 3-dimensional arrays of integers from 0 to 255, of size Width x Height x 3. The 3 represents the three color channels Red, Green, Blue.

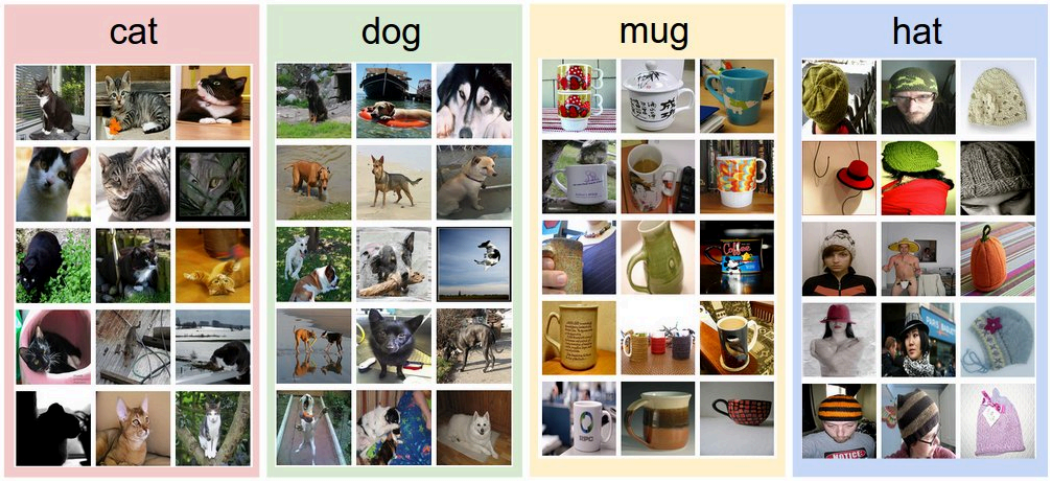
Challenges. Since this task of recognizing a visual concept (e.g. cat) is relatively trivial for a human to perform, it is worth considering the challenges involved from the perspective of a Computer Vision algorithm. As we present (an inexhaustive) list of challenges below, keep in mind the raw representation of images as a 3-D array of brightness values:

- **Viewpoint variation**. A single instance of an object can be oriented in many ways with respect to the camera.
- **Scale variation**. Visual classes often exhibit variation in their size (size in the real world, not only in terms of their extent in the image).
- **Deformation**. Many objects of interest are not rigid bodies and can be deformed in extreme ways.
- **Occlusion**. The objects of interest can be occluded. Sometimes only a small portion of an object (as little as few pixels) could be visible.
- **Illumination conditions**. The effects of illumination are drastic on the pixel level.
- **Background clutter**. The objects of interest may *blend* into their environment, making them hard to identify.
- **Intra-class variation**. The classes of interest can often be relatively broad, such as *chair*. There are many different types of these objects, each with their own appearance.

A good image classification model must be invariant to the cross product of all these variations, while simultaneously retaining sensitivity to the inter-class variations.



Data-driven approach. How might we go about writing an algorithm that can classify images into distinct categories? Unlike writing an algorithm for, for example, sorting a list of numbers, it is not obvious how one might write an algorithm for identifying cats in images. Therefore, instead of trying to specify what every one of the categories of interest look like directly in code, the approach that we will take is not unlike one you would take with a child: we're going to provide the computer with many examples of each class and then develop learning algorithms that look at these examples and learn about the visual appearance of each class. This approach is referred to as a *data-driven approach*, since it relies on first accumulating a *training dataset* of labeled images. Here is an example of what such a dataset might look like:



An example training set for four visual categories. In practice we may have thousands of categories and hundreds of thousands of images for each category.

The image classification pipeline. We've seen that the task in Image Classification is to take an array of pixels that represents a single image and assign a label to it. Our complete pipeline can be formalized as follows:

- **Input**: Our input consists of a set of *N* images, each labeled with one of *K* different classes. We refer to this data as the *training set*.
- **Learning**: Our task is to use the training set to learn what every one of the classes looks like. We refer to this step as *training a classifier*, or *learning a model*.
- **Evaluation**: In the end, we evaluate the quality of the classifier by asking it to predict labels for a new set of images that it has never seen before. We will then compare the true labels of these images to the ones predicted by the classifier. Intuitively, we're hoping that a lot of the predictions match up with the true answers (which we call the *ground truth*).

Linear Classification

In the last section we introduced the problem of Image Classification, which is the task of assigning a single label to an image from a fixed set of categories. Morever, we described the k-Nearest Neighbor (kNN) classifier which labels images by comparing them to (annotated) images from the training set. As we saw, kNN has a number of disadvantages:

- The classifier must *remember* all of the training data and store it for future comparisons with the test data. This is space inefficient because datasets may easily be gigabytes in size.

- Classifying a test image is expensive since it requires a comparison to all training images.

Overview. We are now going to develop a more powerful approach to image classification that we will eventually naturally extend to entire Neural Networks and Convolutional Neural Networks. The approach will have two major components: a **score function** that maps the raw data to class scores, and a **loss function** that quantifies the agreement between the predicted scores and the ground truth labels. We will then cast this as an optimization problem in which we will minimize the loss function with respect to the parameters of the score function.

Parameterized mapping from images to label scores

The first component of this approach is to define the score function that maps the pixel values of an image to confidence scores for each class. We will develop the approach with a concrete example. As before, let's assume a training dataset of images $\boldsymbol{x_i} \in \boldsymbol{R^D}$, each associated with a label $\boldsymbol{y_i}$. Here $\boldsymbol{i = 1 \ldots N}$ and $\boldsymbol{y_i} \in \boldsymbol{1 \ldots K}$. That is, we have **N** examples (each with a dimensionality **D**) and **K** distinct categories. For example, in CIFAR-10 we have a training set of **N** = 50,000 images, each with **D** = 32 x 32 x 3 = 3072 pixels, and **K** = 10, since there are 10 distinct classes (dog, cat, car, etc). We will now define the score function $\boldsymbol{f : R^D \mapsto R^K}$ that maps the raw image pixels to class scores.

Linear classifier. In this module we will start out with arguably the simplest possible function, a linear mapping:

$$\boldsymbol{f(x_i, W, b) = Wx_i + b}$$

In the above equation, we are assuming that the image $\boldsymbol{x_i}$ has all of its pixels flattened out to a single column vector of shape [D x 1]. The matrix **W** (of size [K x D]), and the vector **b** (of size [K x 1]) are the **parameters** of the function. In CIFAR-10, $\boldsymbol{x_i}$ contains all pixels in the i-th image flattened into a single [3072 x 1] column, **W** is [10 x 3072] and **b** is [10 x 1], so 3072 numbers come into the function (the raw pixel values) and 10 numbers come out (the class scores). The parameters in **W** are often called the **weights**, and **b** is called the **bias vector** because it influences the output scores, but without interacting with the actual data $\boldsymbol{x_i}$. However, you will often hear people use the terms *weights* and *parameters* interchangeably.

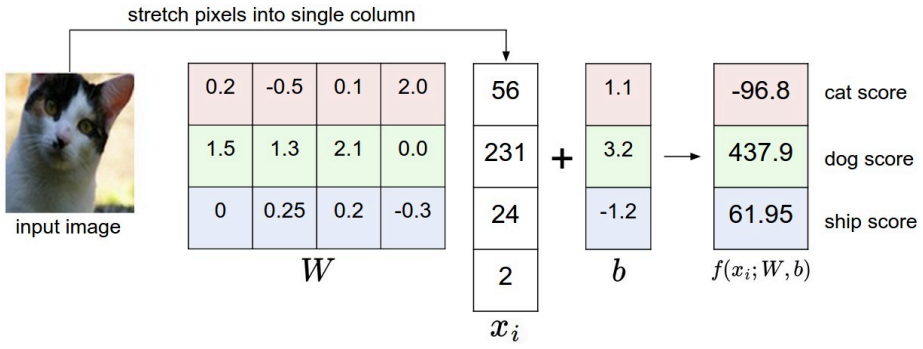
There are a few things to note:

- First, note that the single matrix multiplication $\boldsymbol{Wx_i}$ is effectively evaluating 10 separate classifiers in parallel (one for each class), where each classifier is a row of **W**.
- Notice also that we think of the input data $\boldsymbol{(x_i, y_i)}$ as given and fixed, but we have control over the setting of the parameters **W**,**b**. Our goal will be to set these in such way that the computed scores match the ground truth labels across the whole training set. We will go into much more detail about how this is done, but intuitively we wish that the correct class has a score that is higher than the scores of incorrect classes.
- An advantage of this approach is that the training data is used to learn the parameters **W**,**b**, but once the learning is complete we can discard the entire training set and only keep the learned parameters. That is because a new test image can be simply forwarded through the function and classified based on the computed scores.
- Lastly, note that classifying the test image involves a single matrix multiplication and addition, which is significantly faster than comparing a test image to all training images.

> *Foreshadowing: Convolutional Neural Networks will map image pixels to scores exactly as shown above, but the mapping (f) will be more complex and will contain more parameters.*

Interpreting a linear classifier

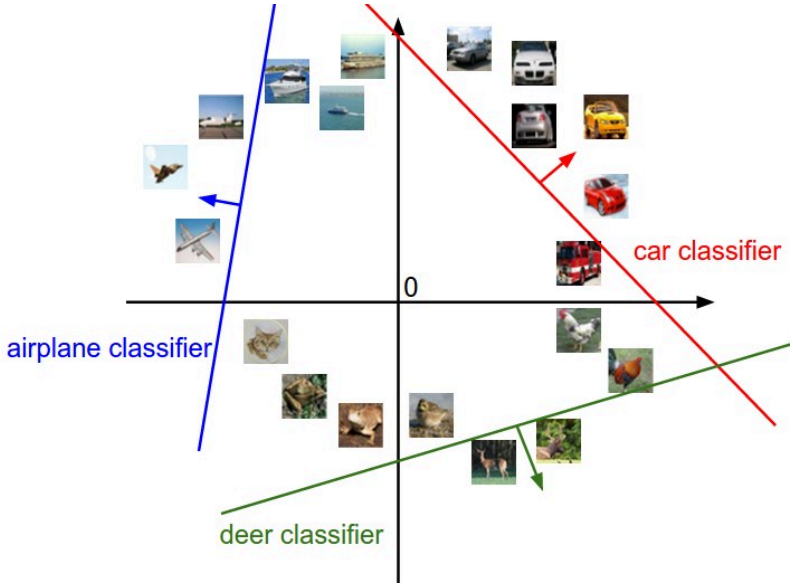
Notice that a linear classifier computes the score of a class as a weighted sum of all of its pixel values across all 3 of its color channels. Depending on precisely what values we set for these weights, the function has the capacity to like or dislike (depending on the sign of each weight) certain colors at certain positions in the image. For instance, you can imagine that the "ship" class might be more likely if there is a lot of blue on the sides of an image (which could likely correspond to water). You might expect that the "ship" classifier would then have a lot of positive weights across its blue channel weights (presence of blue increases score of ship), and negative weights in the red/green channels (presence of red/green decreases the score of ship).



An example of mapping an image to class scores. For the sake of visualization, we assume the image only has 4 pixels (4 monochrome pixels, we are not considering color channels in this example for brevity), and that we have 3 classes (red (cat), green (dog), blue (ship) class). (Clarification: in particular, the colors here simply indicate 3 classes and are not related to the RGB channels.) We stretch the image pixels into a column and perform matrix multiplication to get the scores for each class. Note that this particular set of weights W is not good at all: the weights assign our cat image a very low cat score. In particular, this set of weights seems convinced that it's looking at a dog.

Analogy of images as high-dimensional points. Since the images are stretched into high-dimensional column vectors, we can interpret each image as a single point in this space (e.g. each image in CIFAR-10 is a point in 3072-dimensional space of 32x32x3 pixels). Analogously, the entire dataset is a (labeled) set of points.

Since we defined the score of each class as a weighted sum of all image pixels, each class score is a linear function over this space. We cannot visualize 3072-dimensional spaces, but if we imagine squashing all those dimensions into only two dimensions, then we can try to visualize what the classifier might be doing:



Cartoon representation of the image space, where each image is a single point, and three classifiers are visualized. Using the example of the car classifier (in red), the red line shows all points in the space that get a score of zero for the car class. The red arrow shows the direction of increase, so all points to the right of the red line have positive (and linearly increasing) scores, and all points to the left have a negative (and linearly decreasing) scores.

As we saw above, every row of W is a classifier for one of the classes. The geometric interpretation of these numbers is that as we change one of the rows of W, the corresponding line in the pixel space will rotate in different directions. The biases b, on the other hand, allow our classifiers to translate the lines. In particular, note that without the bias terms, plugging in $x_i = 0$ would always give score of zero regardless of the weights, so all lines would be forced to cross the origin.

Interpretation of linear classifiers as template matching. Another interpretation for the weights W is that each row of W corresponds to a *template* (or sometimes also called a *prototype*) for one of the classes. The score of each class for an image is then obtained by comparing each template with the image using an *inner product* (or *dot product*) one by one to find the one that "fits" best. With this terminology, the linear classifier is doing template matching, where the templates are learned. Another way to think of it is that we are still effectively doing Nearest Neighbor, but instead of having thousands of training images we are only using a single image per class (although we will learn it, and it does not necessarily have to be one of the images in the training set), and we use the (negative) inner product as the distance instead of the L1 or L2 distance.

Skipping ahead a bit: Example learned weights at the end of learning for CIFAR-10. Note that, for example, the ship template contains a lot of blue pixels as expected. This template will therefore give a high score once it is matched against images of ships on the ocean with an inner product.

Additionally, note that the horse template seems to contain a two-headed horse, which is due to both left and right facing horses in the dataset. The linear classifier *merges* these two modes of horses in the data into a single template. Similarly, the car classifier seems to have merged several

modes into a single template which has to identify cars from all sides, and of all colors. In particular, this template ended up being red, which hints that there are more red cars in the CIFAR-10 dataset than of any other color. The linear classifier is too weak to properly account for different-colored cars, but as we will see later neural networks will allow us to perform this task. Looking ahead a bit, a neural network will be able to develop intermediate neurons in its hidden layers that could detect specific car types (e.g. green car facing left, blue car facing front, etc.), and neurons on the next layer could combine these into a more accurate car score through a weighted sum of the individual car detectors.

Bias trick. Before moving on we want to mention a common simplifying trick to representing the two parameters W, b as one. Recall that we defined the score function as:

$$f(x_i, W, b) = Wx_i + b$$

As we proceed through the material it is a little cumbersome to keep track of two sets of parameters (the biases b and weights W) separately. A commonly used trick is to combine the two sets of parameters into a single matrix that holds both of them by extending the vector x_i with one additional dimension that always holds the constant 1 - a default *bias dimension*. With the extra dimension, the new score function will simplify to a single matrix multiply:

$$f(x_i, W) = Wx_i$$

With our CIFAR-10 example, x_i is now [3073 x 1] instead of [3072 x 1] - (with the extra dimension holding the constant 1), and W is now [10 x 3073] instead of [10 x 3072]. The extra column that W now corresponds to the bias b. An illustration might help clarify:

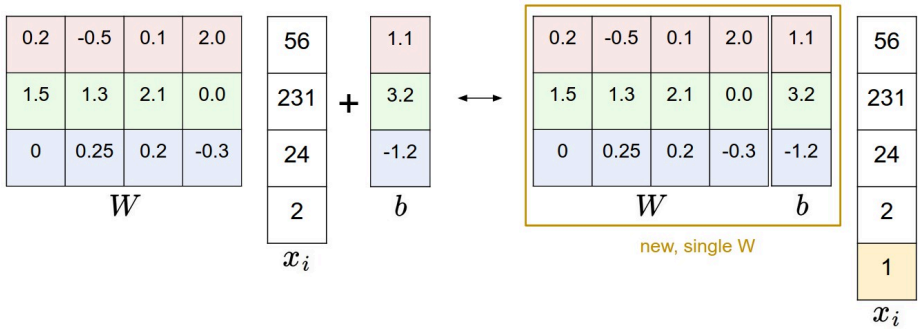


Illustration of the bias trick. Doing a matrix multiplication and then adding a bias vector (left) is equivalent to adding a bias dimension with a constant of 1 to all input vectors and extending the weight matrix by 1 column - a bias column (right). Thus, if we preprocess our data by appending ones to all vectors we only have to learn a single matrix of weights instead of two matrices that hold the weights and the biases.

Image data preprocessing. As a quick note, in the examples above we used the raw pixel values (which range from [0⋯255]). In Machine Learning, it is a very common practice to always perform normalization of your input features (in the case of images, every pixel is thought of as a feature). In particular, it is important to **center your data** by subtracting the mean from every feature. In the case of images, this corresponds to computing a *mean image* across the training images and subtracting it from every image to get images where the pixels range from approximately [-127 ⋯ 127]. Further common preprocessing is to scale each input feature so that its values range from [-1, 1]. Of these, zero mean centering is arguably more important but we will have to wait for its justification until we understand the dynamics of gradient descent.

Loss function

In the previous lecture, we defined a function from the pixel values to class scores, which was parameterized by a set of weights W. Moreover, we saw that we don't have control over the data (x_i, y_i) (it is fixed and given), but we do have control over these weights and we want to set them so that the predicted class scores are consistent with the ground truth labels in the training data.

For example, going back to the example image of a cat and its scores for the classes "cat", "dog" and "ship", we saw that the particular set of weights in that example was not very good at all: We fed in the pixels that depict a cat but the cat score came out very low (-96.8) compared to the other classes (dog score 437.9 and ship score 61.95). We are going to measure our unhappiness with outcomes such as this one with a **loss function** (or sometimes also referred to as the **cost function** or the **objective**). Intuitively, the loss will be high if we're doing a poor job of classifying the training data, and it will be low if we're doing well.

Softmax classifier

There are several ways to define the details of the loss function. As a first example we will first develop a commonly used loss called the **Softmax classifier**. If you've heard of the binary Logistic Regression classifier before, the Softmax classifier is its generalization to multiple classes. The Softmax classifier gives an intuitive output (normalized class probabilities) and also has a probabilistic interpretation that we will describe shortly. In the Softmax classifier, the function mapping $f(x_i; W) = Wx_i$ stays unchanged, but we now interpret these scores as the unnormalized log probabilities for each class and use a **cross-entropy loss** that has the form:

$$L_i = -\log\left(\frac{e^{f_{y_i}}}{\sum_j e^{f_j}}\right) \qquad \text{or equivalently} \qquad L_i = -f_{y_i} + \log\sum_j e^{f_j}$$

where we are using the notation f_j to mean the j-th element of the vector of class scores f. As before, the full loss for the dataset is the mean of L_i over all training examples together with a regularization term $R(W)$. The function $f_j(z) = \frac{e^{z_j}}{\sum_k e^{z_k}}$ is called the **softmax function**: It takes a vector of arbitrary real-valued scores (in z) and squashes it to a vector of values between zero and one that sum to one. The full cross-entropy loss that involves the softmax function might look scary if you're seeing it for the first time but it is relatively easy to motivate.

Information theory view. The *cross-entropy* between a "true" distribution p and an estimated distribution q is defined as:

$$H(p, q) = -\sum_x p(x) \log q(x)$$

The Softmax classifier is hence minimizing the cross-entropy between the estimated class probabilities ($q = e^{f_{y_i}} / \sum_j e^{f_j}$ as seen above) and the "true" distribution, which in this interpretation is the distribution where all probability mass is on the correct class (i.e. $p = [0, \ldots 1, \ldots, 0]$ contains a single 1 at the y_i -th position.). Moreover, since the cross-entropy can be written in terms of entropy and the Kullback-Leibler divergence as $H(p, q) = H(p) + D_{KL}(p||q)$, and the entropy of the delta function p is zero, this is also

equivalent to minimizing the KL divergence between the two distributions (a measure of distance). In other words, the cross-entropy objective *wants* the predicted distribution to have all of its mass on the correct answer.

Probabilistic interpretation. Looking at the expression, we see that

$$P(y_i \mid x_i; W) = \frac{e^{f_{y_i}}}{\sum_j e^{f_j}}$$

can be interpreted as the (normalized) probability assigned to the correct label y_i given the image x_i and parameterized by W. To see this, remember that the Softmax classifier interprets the scores inside the output vector f as the unnormalized log probabilities. Exponentiating these quantities therefore gives the (unnormalized) probabilities, and the division performs the normalization so that the probabilities sum to one. In the probabilistic interpretation, we are therefore minimizing the negative log likelihood of the correct class, which can be interpreted as performing *Maximum Likelihood Estimation* (MLE). A nice feature of this view is that we can now also interpret the regularization term $R(W)$ in the full loss function as coming from a Gaussian prior over the weight matrix W, where instead of MLE we are performing the *Maximum a posteriori* (MAP) estimation. We mention these interpretations to help your intuitions, but the full details of this derivation are beyond the scope of this class.

Practical issues: Numeric stability. When you're writing code for computing the Softmax function in practice, the intermediate terms $e^{f_{y_i}}$ and $\sum_j e^{f_j}$ may be very large due to the exponentials. Dividing large numbers can be numerically unstable, so it is important to use a normalization trick. Notice that if we multiply the top and bottom of the fraction by a constant C and push it into the sum, we get the following (mathematically equivalent) expression:

$$\frac{e^{f_{y_i}}}{\sum_j e^{f_j}} = \frac{Ce^{f_{y_i}}}{C\sum_j e^{f_j}} = \frac{e^{f_{y_i}+\log C}}{\sum_j e^{f_j+\log C}}$$

We are free to choose the value of C. This will not change any of the results, but we can use this value to improve the numerical stability of the computation. A common choice for C is to set $\log C = -\max_j f_j$. This simply states that we should shift the values inside the vector f so that the highest value is zero. In code:

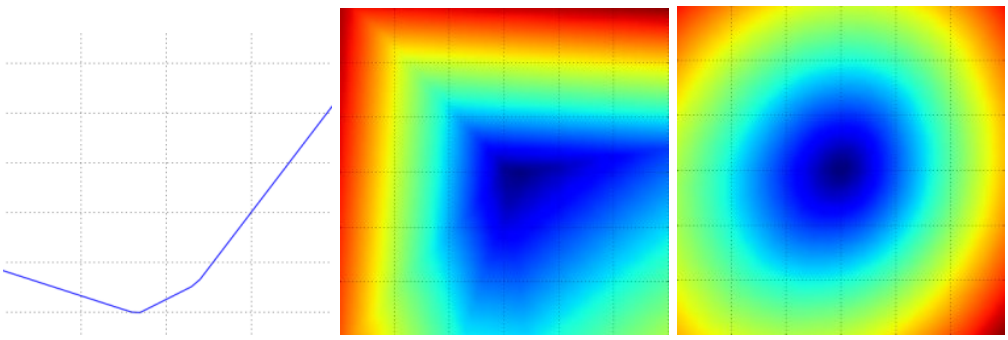
```
f = np.array([123, 456, 789]) # example with 3 classes and each having large scores
p = np.exp(f) / np.sum(np.exp(f)) # Bad: Numeric problem, potential blowup

# instead: first shift the values of f so that the highest number is 0:
f -= np.max(f) # f becomes [-666, -333, 0]
p = np.exp(f) / np.sum(np.exp(f)) # safe to do, gives the correct answer
```

Possibly confusing naming conventions. To be precise, the *Softmax classifier* uses the *cross-entropy loss*. The Softmax classifier gets its name from the *softmax function*, which is used to squash the raw class scores into normalized positive values that sum to one, so that the cross-entropy loss can be

applied. In particular, note that technically it doesn't make sense to talk about the "softmax loss", since softmax is just the squashing function, but it is a relatively commonly used shorthand.

Visualizing the loss function

The loss functions we'll look at in this class are usually defined over very high-dimensional spaces (e.g. in CIFAR-10 a linear classifier weight matrix is of size [10 x 3073] for a total of 30,730 parameters), making them difficult to visualize. However, we can still gain some intuitions about one by slicing through the high-dimensional space along rays (1 dimension), or along planes (2 dimensions). For example, we can generate a random weight matrix W (which corresponds to a single point in the space), then march along a ray and record the loss function value along the way. That is, we can generate a random direction W_1 and compute the loss along this direction by evaluating $L(W + aW_1)$ for different values of a. This process generates a simple plot with the value of a as the x-axis and the value of the loss function as the y-axis. We can also carry out the same procedure with two dimensions by evaluating the loss $L(W + aW_1 + bW_2)$ as we vary a, b. In a plot, a, b could then correspond to the x-axis and the y-axis, and the value of the loss function can be visualized with a color:



Loss function landscape for the Multiclass SVM (without regularization) for one single example (left,middle) and for a hundred examples (right) in CIFAR-10. Left: one-dimensional loss by only varying **a**. Middle, Right: two-dimensional loss slice, Blue = low loss, Red = high loss. Notice the piecewise-linear structure of the loss function. The losses for multiple examples are combined with average, so the bowl shape on the right is the average of many piece-wise linear bowls (such as the one in the middle).

Optimization

In the last lecture and in the previous section, we introduced two key components in context of the image classification task:

1. A (parameterized) **score function** mapping the raw image pixels to class scores (e.g. a linear function)
2. A **loss function** that measured the quality of a particular set of parameters based on how well the induced scores agreed with the ground truth labels in the training data. We saw that there are many ways and versions of this (e.g. Softmax).

We are now going to introduce the third and last key component: **optimization**. Optimization is the process of finding the set of parameters W that minimize the loss function.

Foreshadowing: Once we understand how these three core components interact, we will revisit the first component (the parameterized function mapping) and extend it to functions much more complicated than a linear mapping: First entire Neural Networks, and then Convolutional Neural Networks. The loss functions and the optimization process will remain relatively unchanged.

To reiterate, the loss function lets us quantify the quality of any particular set of weights **W**. The goal of optimization is to find **W** that minimizes the loss function. We will now motivate and slowly develop an approach to optimizing the loss function. For those of you coming to this class with previous experience, this section might seem odd since the working example we'll use (the SVM loss) is a convex problem, but keep in mind that our goal is to eventually optimize Neural Networks where we can't easily use any of the tools developed in the Convex Optimization literature.

Core Idea: Following the Gradient

In the previous section we tried to find a direction in the weight-space that would improve our weight vector (and give us a lower loss). It turns out that there is no need to randomly search for a good direction: we can compute the *best* direction along which we should change our weight vector that is mathematically guaranteed to be the direction of the steepest descend (at least in the limit as the step size goes towards zero). This direction will be related to the **gradient** of the loss function. In our hiking analogy, this approach roughly corresponds to feeling the slope of the hill below our feet and stepping down the direction that feels steepest.

In one-dimensional functions, the slope is the instantaneous rate of change of the function at any point you might be interested in. The gradient is a generalization of slope for functions that don't take a single number but a vector of numbers. Additionally, the gradient is just a vector of slopes (more commonly referred to as **derivatives**) for each dimension in the input space. The mathematical expression for the derivative of a 1-D function with respect its input is:

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

When the functions of interest take a vector of numbers instead of a single number, we call the derivatives **partial derivatives**, and the gradient is simply the vector of partial derivatives in each dimension.

Computing the gradient

There are two ways to compute the gradient: A slow, approximate but easy way (**numerical gradient**), and a fast, exact but more error-prone way that requires calculus (**analytic gradient**). We will now present both.

Computing the gradient numerically with finite differences

The formula given above allows us to compute the gradient numerically. Here is a generic function that takes a function `f`, a vector `x` to evaluate the gradient on, and returns the gradient of `f` at `x`:

```
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
```

Following the gradient formula we gave above, the code above iterates over all dimensions one by one, makes a small change `h` along that dimension and calculates the partial derivative of the loss function along that dimension by seeing how much the function changed. The variable `grad` holds the full gradient in the end.

Practical considerations. Note that in the mathematical formulation the gradient is defined in the limit as **h** goes towards zero, but in practice it is often sufficient to use a very small value (such as 1e-5 as seen in the example). Ideally, you want to use the smallest step size that does not lead to numerical issues. Additionally, in practice it often works better to compute the numeric gradient using the **centered difference formula**: $[f(x+h) - f(x-h)]/2h$. See wiki for details.

We can use the function given above to compute the gradient at any point and for any function. Lets compute the gradient for the CIFAR-10 loss function at some random point in the weight space:

```
# to use the generic code above we want a function that takes a single argument
# (the weights in our case) so we close over X_train and Y_train
def CIFAR10_loss_fun(W):
  return L(X_train, Y_train, W)
```

```
W = np.random.rand(10, 3073) * 0.001 # random weight vector
df = eval_numerical_gradient(CIFAR10_loss_fun, W) # get the gradient
```

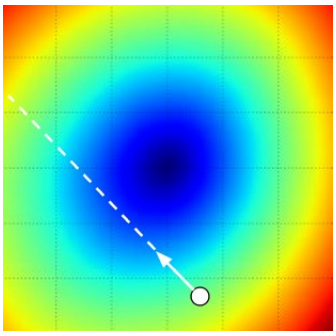
The gradient tells us the slope of the loss function along every dimension, which we can use to make an update:

```
loss_original = CIFAR10_loss_fun(W) # the original loss
print 'original loss: %f' % (loss_original, )

# lets see the effect of multiple step sizes
for step_size_log in [-10, -9, -8, -7, -6, -5,-4,-3,-2,-1]:
  step_size = 10 ** step_size_log
  W_new = W - step_size * df # new position in the weight space
  loss_new = CIFAR10_loss_fun(W_new)
  print 'for step size %f new loss: %f' % (step_size, loss_new)

# prints:
# original loss: 2.200718
# for step size 1.000000e-10 new loss: 2.200652
# for step size 1.000000e-09 new loss: 2.200057
# for step size 1.000000e-08 new loss: 2.194116
# for step size 1.000000e-07 new loss: 2.135493
# for step size 1.000000e-06 new loss: 1.647802
# for step size 1.000000e-05 new loss: 2.844355
# for step size 1.000000e-04 new loss: 25.558142
# for step size 1.000000e-03 new loss: 254.086573
# for step size 1.000000e-02 new loss: 2539.370888
# for step size 1.000000e-01 new loss: 25392.214036
```

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

Effect of step size. The gradient tells us the direction in which the function has the steepest rate of increase, but it does not tell us how far along this direction we should step. As we will see later in the course, choosing the step size (also called the *learning rate*) will become one of the most important (and most headache-inducing) hyperparameter settings in training a neural network. In our blindfolded hill-descent analogy, we feel the hill below our feet sloping in some direction, but the step length we should take is uncertain. If we shuffle our feet carefully we can expect to make consistent but very small progress (this corresponds to having a small step size). Conversely, we can choose to make a large, confident step in an attempt to descend faster, but this may not pay off. As you can see in the code example above, at some point taking a bigger step gives a higher loss as we "overstep".

Visualizing the effect of step size. We start at some particular spot W and evaluate the gradient (or rather its negative - the white arrow) which tells us the direction of the steepest decrease in the loss function. Small steps are likely to lead to consistent but slow progress. Large steps can lead to better progress but are more



risky. Note that eventually, for a large step size we will overshoot and make the loss worse. The step size (or as we will later call it - the **learning rate**) will become one of the most important hyperparameters that we will have to carefully tune.

A problem of efficiency. You may have noticed that evaluating the numerical gradient has complexity linear in the number of parameters. In our example we had 30730 parameters in total and therefore had to perform 30,731 evaluations of the loss function to evaluate the gradient and to perform only a single parameter update. This problem only gets worse, since modern Neural Networks can easily have tens of millions of parameters. Clearly, this strategy is not scalable and we need something better.

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* goes to zero), 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.

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:

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

where 1 is the indicator function that is one if the condition inside is true or zero otherwise. While the expression may look scary when it is written out, when you're implementing this in code you'd simply count the number of classes that didn't meet the desired margin (and hence contributed to the loss function) and then the data vector x_i scaled by this number is the gradient. Notice that this is the gradient only with respect to the row of W that corresponds to the correct class. For the other rows where $j \neq y_i$ the gradient is:

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

Once you derive the expression for the gradient it is straight-forward to implement the expressions and use them to perform the gradient update.

Gradient Descent

Now that we can compute the gradient of the loss function, the procedure of repeatedly evaluating the gradient and then performing a parameter update is called *Gradient Descent*. Its **vanilla** version looks as follows:

```
# Vanilla Gradient Descent

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

This simple loop is at the core of all Neural Network libraries. There are other ways of performing the optimization (e.g. LBFGS), but Gradient Descent is currently by far the most common and established way of optimizing Neural Network loss functions. Throughout the class we will put some bells and whistles on the details of this loop (e.g. the exact details of the update equation), but the core idea of following the gradient until we're happy with the results will remain the same.

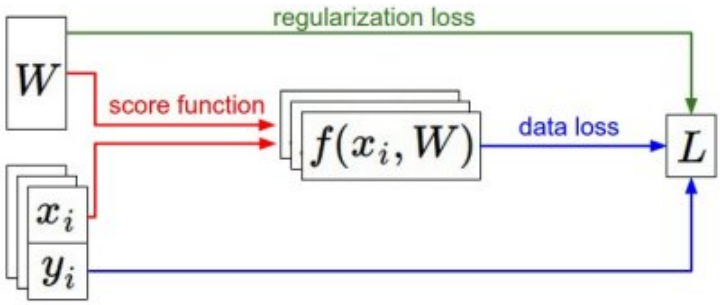
Mini-batch gradient descent. In large-scale applications (such as the ILSVRC challenge), the training data can have on order of millions of examples. Hence, it seems wasteful to compute the full loss function over the entire training set in order to perform only a single parameter update. A very common approach to addressing this challenge is to compute the gradient over **batches** of the training data. For example, in current state of the art ConvNets, a typical batch contains 256 examples from the entire training set of 1.2 million. This batch is then used to perform a parameter update:

```
# 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
```

The reason this works well is that the examples in the training data are correlated. To see this, consider the extreme case where all 1.2 million images in ILSVRC are in fact made up of exact duplicates of only 1000 unique images (one for each class, or in other words 1200 identical copies of each image). Then it is clear that the gradients we would compute for all 1200 identical copies would all be the same, and when we average the data loss over all 1.2 million images we would get the exact same loss as if we only evaluated on a small subset of 1000. In practice of course, the dataset would not contain duplicate images, the gradient from a mini-batch is a good approximation of the gradient of the full objective. Therefore, much faster convergence can be achieved in practice by evaluating the mini-batch gradients to perform more frequent parameter updates.

The extreme case of this is a setting where the mini-batch contains only a single example. This process is called **Stochastic Gradient Descent (SGD)** (or also sometimes **on-line** gradient descent). This is relatively less common to see because in practice due to vectorized code optimizations it can be computationally much more efficient to evaluate the gradient for 100 examples, than the gradient for one example 100 times. Even though SGD technically refers to using a single example at a time to evaluate the gradient, you will hear people use the term SGD even when referring to mini-batch gradient descent (i.e. mentions of MGD for "Minibatch Gradient Descent", or BGD for "Batch gradient descent" are rare to see), where it is usually assumed that mini-batches are used. The size of the mini-batch is a hyperparameter but it is not very common to cross-validate it. It is usually based on memory constraints (if any), or set to some value, e.g. 32, 64 or 128. We use powers of 2 in practice because many vectorized operation implementations work faster when their inputs are sized in powers of 2.

Summary of the Information Flow



The dataset of pairs of **(x,y)** is given and fixed. The weights start out as random numbers and can change. During the forward pass the score function computes class scores, stored in vector **f**. The loss function contains two components: The data loss computes the compatibility between the scores **f** and the labels **y**. The regularization loss is only a function of the weights. During Gradient Descent, we compute the gradient on the weights (and optionally on data if we wish) and use them to perform a parameter update during Gradient Descent.