Why Kernels?
For classification tasks, it is often the case that the optimal decision boundary is a nonlinear function. In these cases, linear classifiers can explore the data's separability in an alternative feature space using kernel functions. Kernel functions, which map two points in the input space to a real number, each correspond to the inner product of two feature maps in some unique feature space (known as a Reproducing Kernel Hilbert Space). That is,

$$K(x, x') = \langle \Phi(x), \Phi(x') \rangle$$

It turns out that the solution to many learning problems can be written as a linear combination of the kernel function at the training set points. That is, for the problem of minimizing the (convex and continuous) empirical risk,

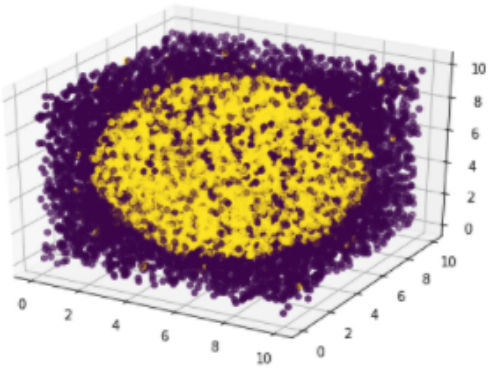
$$\inf_{f \in \mathcal{H}} \hat{\mathcal{E}}(f) + \lambda ||f||_{\mathcal{H}}||^2,$$

the optimal function $\hat{f}$ can be written as

$$\hat{f}(x) = \sum_{i}^{n} K(x, x_i) c_i$$

What is even more interesting is that we can discover the weights c using gradient descent without ever invoking the feature map Φ the corresponds to the kernel function K. Indeed in some cases, the feature map represented by K may even be of infinite dimension (the gaussian kernel, for example).

In this way, kernel functions allow us to transform the problem into a more separable space and still bypass the need for an explicit feature map. Kernel logistic regression does precisely this. For example, if we consider the 3D data set represented here:



we will discover that a gaussian kernel is a much better performer than say, the linear kernel. It goes without saying that even if in this simple case we could encode an intelligent feature map ourselves without invoking kernels, for larger problems that is more difficult to do.

Gradient Descent for Kernel Logistic Regression
For standard logistic regression, recall that for input matrix X and labels y, we aim to minimize the log-likelihood of the data, with regularization, given our weight vector w:

$$\min_w \frac{1}{n}\left[\sum_{i|y_i=1}^{n} \log\left(\frac{1}{1+e^{-y_i\langle w,x_i\rangle}}\right) + \sum_{i|y_i=0}^{n} \log\left(1-\frac{1}{1+e^{-y_i\langle w,x_i\rangle}}\right)\right] + \lambda||w||^2,$$

which can be done via gradient descent:

$$w_0 = 0, \quad w_{t+1}^j = w_t^j - \gamma\left(\sum_i (y_i - \frac{1}{1+e^{y_i\langle w,x_i\rangle}})x_i^j + 2\lambda w_t^j\right)$$

For kernel logistic regression, the gradient descent iteration becomes:

$$c \leftarrow c + \gamma\left(y - \frac{1}{1+e^{\hat{K}c}} + 2\lambda c\right),$$

where $\hat{K}$ is the n by n kernel matrix consisting of the kernel function applied to each pair of training set points.

Conveniently, this does not depend on feature map Φ.

Using This Package

This package offers 3 types of gradient descent for solving kernel logistic regression: batch, stochastic, and mini-batch gradient descent. Let's briefly discuss the pros and cons of each.

Stochastic Gradient Descent
Stochastic gradient descent updates the weight vector by choosing a random example from the data set and calculating the error. The main advantage of this approach is two-fold: 1) it can be used in online settings, where data is acquired or revealed piece by piece, and 2) for non-convex loss functions, it can avoid local minima (not a worry with logistic regression). Drawbacks include a longer run time due to such frequent updates of the model, and a

noisier gradient signal resulting in a higher variance of the model parameters during training.

For kernel logistic regression, the stochastic gradient descent iteration is given by:

$$c_i \leftarrow c_i + \gamma \left(y_i - \frac{1}{1 + e^{(\hat{K}c)_i}} + 2\lambda c_i \right)$$

The vector $\hat{K}c$ can be cleverly updated in linear time without recomputing the product each time.

Batch Gradient Descent
Batch gradient descent only updates the model after having seen all of the data points. In this way, it is usually more computationally efficient and more stable than its random cousin, but it may converge on a local minimum, and it often relies on the entire matrix being stored in memory. To boot, training time for batch descent can be very slow on large datasets.

Mini-batch Gradient Descent
Mini-batch gradient descent, a growing favorite of many, attempts to capture the best of both worlds. It randomly selects a batch-size number of points to update the model. The batch size may slide between 1 (stochastic) and n (batch), but usually a good choice is on the order of 30. It tries not to converge too slowly like batch, while simultaneously avoid the noise associated with a purely stochastic gradient descent. As a drawback, the batch size parameter may need to be tuned during validation.