

Two Sample  
Discrimination

Chandi  
Bhandari,  
Rahul Kumar,  
Brian  
Robinson, and  
Simon  
Stolarczyk

Gretton et. al.  
RKHS method

# How do you tell when two samples come from different distributions?

Chandi Bhandari, Rahul Kumar, Brian Robinson, and Simon Stolarczyk

December 1, 2015

# Motivating Scenario

## Two Sample Discrimination

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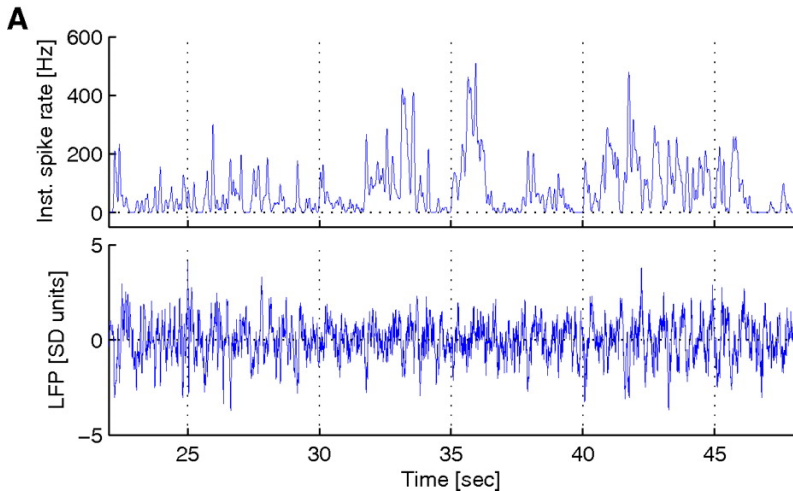


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From Gretton et. al.

In bioinformatics, it is of interest to compare microarray data from identical tissue types as measured by different laboratories, to detect whether the data may be analysed jointly, or whether differences in experimental procedure have caused systematic differences in the data distributions.

# Basic Question

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Given two distributions  $p$  and  $q$ , how do we test whether they are different on the basis of samples drawn from each of them?

$X = (X^1, \dots, X^m)$  drawn from  $p$

$Y = (Y^1, \dots, Y^n)$  drawn from  $q$

# Basic Plotting

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Useful for lower dimensional data, but how do we visualize the difference when  $p = N_d(\mu, I)$  when  $d \gg 3$ ?

# Permuation Testing

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See book info as well as

<http://stats.stackexchange.com/questions/59774/test-whether-variables-follow-the-same-distribution>

# Kolmogorov-Smirnov Test

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# Motivating Fact

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Expectations over all continuous functions can distinguish probability distributions:

$$p = q \text{ iff. } E_p[f(x)] = E_q[f(y)] \quad \forall f \in C(X)$$

# Mean Maximum Discrepancy

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For a set of functions  $\mathcal{F}$  define

$$\text{MMD}[\mathcal{F}, p, q] = \sup_{f \in \mathcal{F}} (E_p[f(x)] - E_q[f(y)])$$

# MMD Estimator

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$$MMD_b[\mathcal{F}, p, q] = \sup_{f \in \mathcal{F}} \left( \frac{1}{m} \sum_{i=1}^m f(x_i) - \frac{1}{n} \sum_{i=1}^n f(y_i) \right)$$

# How to choose $\mathcal{F}$

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We need something computationally feasible. We want our space  $\mathcal{F}$  to be a Hilbert Space with the nice property that taking the expectation of any function is the same as the inner product with some special function

$$E_x f = \langle f, \mu_p \rangle_{\mathcal{H}}$$

and we want

$$k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}$$

# Estimator

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$$\begin{aligned} MMD_u^2[\mathcal{F}, X, Y] = & \frac{1}{m(m-1)} \sum_{i=1}^m \sum_{j \neq i}^m k(x_i, x_j) \\ & + \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i}^n k(y_i, y_j) \\ & - \frac{2}{mn} \sum_{i=1}^m \sum_{j=1}^n k(x_i, y_j) \end{aligned}$$

# Linear Estimator

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$$MMD_l^2[\mathcal{F}, X, Y] = \frac{2}{m} \sum_{i=1}^{m/2} h((x_{2i-1}, y_{2i-1}), (x_{2i}, y_{2i}))$$

where

$$z \sim (x, y), h(z_i, z_j) := k(x_i, x_j) + k(y_i, y_j) - k(x_i, y_j) - k(x_j, y_i)$$

# Applying the tests to artificially generated data

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# Apply the test to experimental data

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- Medical data
- The distributions for connections on a graph.
- other from Dr. Fu