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

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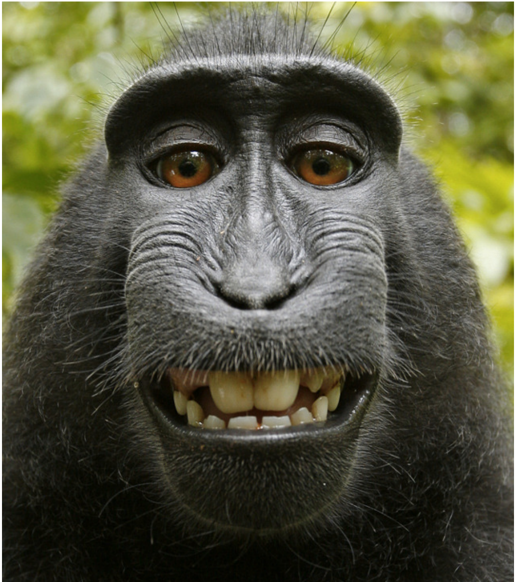
Motivating Scenario



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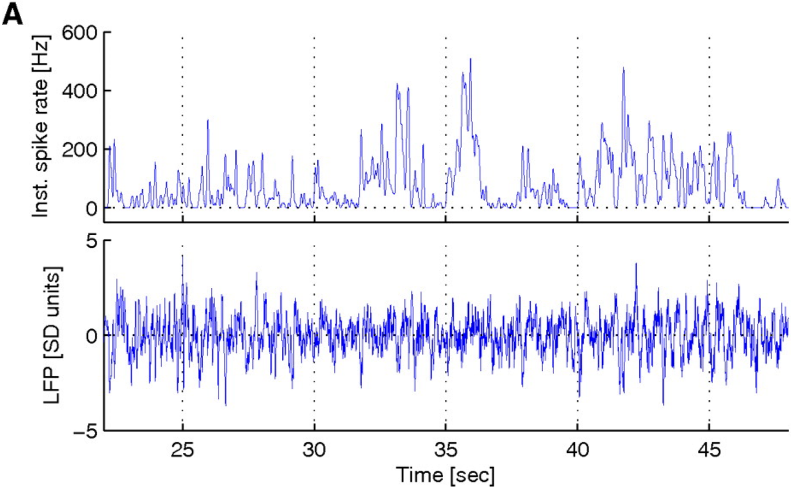

Basic Question

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

$$X = (X^1, ..., X^m) \text{ drawn from } p$$

$$Y = (Y^1, ..., Y^n) \text{ drawn from } q$$

Example

$$X = (1.4110420, -0.6491983, -0.2034312, ..., 0.5670504)$$

$$Y = (2.10555009, 1.59182751, 0.85874229, ..., 0.38632577)$$

Example

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$$H_0 : p = q$$

Basic Plotting

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

Permutation Testing

- Develop a statistic given the samples.
- Permute the samples and run the statistic again.
- See where the original statistic falls on a plot of the statistic for different permutations.

Kolmogorov-Smirnov Test

Motivating Fact

Expectations over all continuous functions can distinguish probability distributions:

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

Mean Maximum Discrepancy

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

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

MMD Estimator

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

How to choose $\mathcal{F}$

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

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

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

Apply the test to experimental data

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