Topics in Two-Sample Testing

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(joint work with Susan Holmes)

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Outline

- Motivation: breast cancer study with heterogeneous data
- Friedman's two-sample test [?]: leverage regression and classification techniques
- Univariate data and linear scoring functions: permutation t-test
- Permutation dependence: Stein's method for rates of convergence bounds
- Simulations to verify bounds in proof (experimental mathematics)
- Kernel-based two sample tests for non-vectorial data
- Multiple Kernel Learning for heterogeneous data

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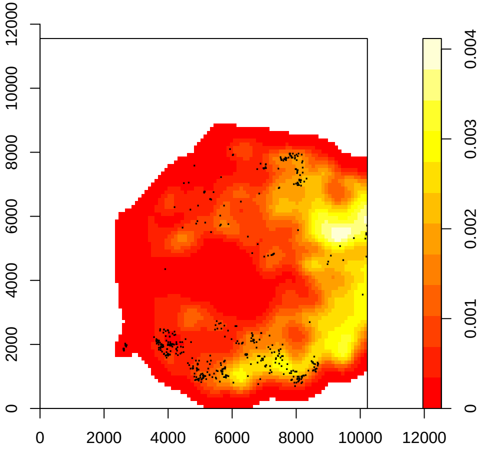
Breast Cancer Data: Spatial



Breast Cancer Data: Survival

Pathology no.	Initial Diagnosis Date	Relapse or Disease Free	RDF (R=relapsed; F=DF)	Recurrence Date	Las
98_17969D	1997-08-25	Disease Free	F	Disease Free	
97_24046C8	1997-08-25	Disease Free	F	Disease Free	
98_8501C1	1998-04-03	Disease Free	F	Disease Free	
98_8501A1	1998-04-03	Disease Free	F	Disease Free	
98_9134D4	1998-04-09	Left in-situ BrCa in 1999 (2nd primary cancer, not a metastasis from the right BrCa in 1997)	F	Disease Free	
98_9134B	1998-04-09	Left in-situ BrCa in 1999 (2nd primary cancer, not a metastasis from the right BrCa in 1997)	F	Disease Free	
98_14783B1	1998-06-10	bone, brain, lymph nodes, pericardium, liver metastasis	R	2004-07-30	
98_14783A	1998-06-10	bone, brain, lymph nodes, pericardium, liver metastasis	R	2004-07-30	
98_16169C2	1998-06-24	Disease Free	F	Disease Free	
98_16169A	1998-06-24	Disease Free	F	Disease Free	
98_16169B	1998-06-24	Disease Free	F	Disease Free	
98_16253C1	1998-06-25	Disease Free	F	Disease Free	
60C1	1998-07-10	Disease Free	F	Disease Free	

Breast Cancer Data: Medical

Pathology no.	Age at time of diagnosis	Gender	SLN tumor status	Diagnosis	ER status	PR status	Her-2 overexpressio
98_17969D	68	F	+	Invasive ductal carcinoma (IDC)	-	-	-
97_24046C8	68	F	+	Invasive ductal carcinoma (IDC)	-	-	-
98_8501C1	51	F	+	IDC & DCIS	+	+	?
98_8501A1	51	F	+	IDC & DCIS	+	+	?
98_9134D4	70	F	+	IDC	+	+	n/a
98_9134B	70	F	+	IDC	+	+	n/a
98_14783B1	67	F	+	IDC & DCIS	+	+	+
98_14783A	67	F	+	IDC & DCIS	+	+	+
98_16169C2	79	F	+mic	IDC	+	+	+
98_16169A	79	F	+mic	IDC	+	+	+
98_16169B	79	F	+mic	IDC	+	+	+
98_16253C1	70	F	+mic	IDC & DCIS	+	-	-
60C1	51	F	- (rare keratin+ cells)	IDC & DCIS	+	+	+
				IDC; DCIS;			

Breast Cancer Study

- How do you deal with the data integration problem?
- Kernel methods
- Are there any differences (spatial, medical) between women who relapse and those who remain disease free?
- Two-sample tests

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Friedman's Two-Sample Test

$\{\mathbf{x}_i\}_1^N$ from $p(\mathbf{x})$ and $\{\mathbf{z}_i\}_1^M$ from $q(\mathbf{z})$ testing
$\mathcal{H}_A$: $p \neq q$ against $\mathcal{H}_0$: $p = q$

1. Pool the two samples $\{\mathbf{u}_i\}_1^{N+M} = \{\mathbf{x}_i\}_1^N \cup \{\mathbf{z}_i\}_1^M$.
2. Assign label $y_i = 1$ to the first group and $y_i = -1$ to the second group.
3. Apply a binary classification learning machine f to the training data to score the observations $\{s_i = f(\mathbf{u}_i)\}_1^{N+M}$.
4. Calculate a univariate two-sample test statistic $T = T(\{s_i\}_1^N, \{s_i\}_{N+1}^{N+M})$.
5. Determine the permutation null distribution of the above statistic to yield a p-value.

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Permutation t-test Connection

With univariate data and linear scoring functions/kernels, Friedman's test reduces to the permutation t-test (normal convergence result). With multivariate/non-vectorial/heterogeneous data and arbitrary kernels, null distribution is consistent with the Normal.

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Other Work

- Fisher (1935) [**?**] proposed distribution-free randomization test.
- Lehmann [**?**] proved a normal convergence result for the randomization distribution.
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Stein's Method and the Randomization Distribution

Let $\Phi(t)$ denote the standard normal CDF.
Can we get a bound on

$$\sup_{t \in \mathbb{R}} |P(T \leq t) - \Phi(t)|?$$

$\mathcal{O}(N^{-1/4})$ with mild conditions on the data and $\mathcal{O}(N^{-1/2})$ with an additional condition

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Other Results

Theorem (Berry-Esseen)

Suppose $X_1, \ldots, X_n$ are i.i.d. random variables with $\mathbb{E}X_i = 0$, $\mathbb{E}X_i^2 = \sigma^2 > 0$, and $\mathbb{E}|X_i|^3 = \rho < \infty$. Let $F_n(x)$ denote the CDF of standardized sample mean of the X_i. Then

$$\sup_x |F_n(x) - \Phi(x)| \leq \frac{0.33477(\rho + 0.429\sigma^3)}{\sigma^3\sqrt{n}}$$

$$= \frac{C}{\sqrt{n}} f(\rho, \sigma).$$

Note that ρ and σ are fixed as $n \to \infty$.

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Theorem (Hoeffding, Stein)

Let $A = \{a_{ij}\}_{i,j \in \{1,\dots,n\}}$ be a square array of numbers such that $\sum_j a_{ij} = 0$ for all i, $\sum_i a_{ij} = 0$ for all j, and $\sum_i \sum_j a_{ij}^2 = n-1$. Then with $F_n(x) = P(\sum_i a_{i\Pi(i)} \le x)$,

$$|F_n(x) - \Phi(x)| \le \frac{C}{\sqrt{n}} \left(\sqrt{\sum_{i,j} a_{ij}^4} + \sqrt{\sum_{i,j} |a_{ij}|^3} \right)$$
$$= \frac{C}{\sqrt{n}} f(A).$$

Given a sampling scheme for A, $f(A)$ must be $\mathcal{O}(1)$ to have rate $\mathcal{O}(n^{-1/2})$.

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Exchangeable Pair

Assume $M = N$. Fix data $\{u_1, \ldots, u_N, u_{N+1}, \ldots, u_{2N}\}$. Π is a uniformly random permutation, and let

$$T = T\left(\{u_{\Pi(i)}\}_{i=1}^{N}, \{u_{\Pi(i)}\}_{i=N+1}^{2N}\right).$$

Let $(I, J) = (i, j)$ w.p. $\frac{1}{N^2}$ for $1 \leq i \leq N$ and $N+1 \leq j \leq 2N$. Then

$$T' = T\left(\{u_{\Pi \circ (I,J)(i)}\}_{i=1}^{N}, \{u_{\Pi \circ (I,J)(i)}\}_{i=N+1}^{2N}\right).$$

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Main Theorem

Theorem

If T, T' are mean 0, exchangeable random variables with variance $\mathbb{E}[T^2]$ satisfying

$$\mathbb{E}[T' - T | T] = -\lambda(T - R)$$

for some $\lambda \in (0,1)$ and some random variable R, then $\sup_{t\in\mathbb{R}} |P(T \le t) - \Phi(t)|$ *is bounded by*

$$\underbrace{(2\pi)^{-1/4}\sqrt{\frac{\mathbb{E}|T' - T|^3}{\lambda}}}_{\le N^{-1/4} f_1(\mathbf{u})} + \underbrace{\frac{1}{2\lambda}\sqrt{\mathrm{var}(\mathbb{E}[(T' - T)^2 | T])}}_{\le N^{-1} f_2(\mathbf{u})}$$

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Main Theorem (Improved Rate)

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If in addition $|T' - T| \leq \delta$, $\sup_{t \in \mathbb{R}} |P(T \leq t) - \Phi(t)|$ *is bounded by*

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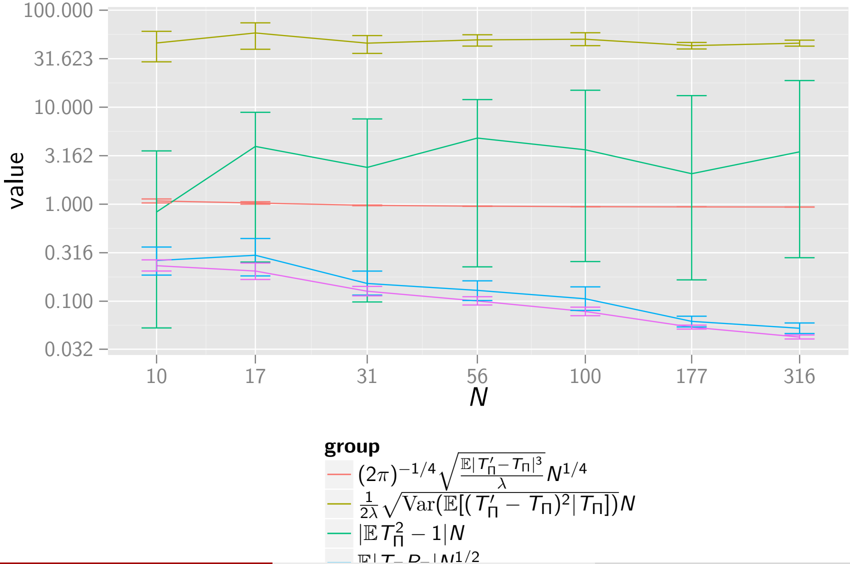
Simulated Bounds



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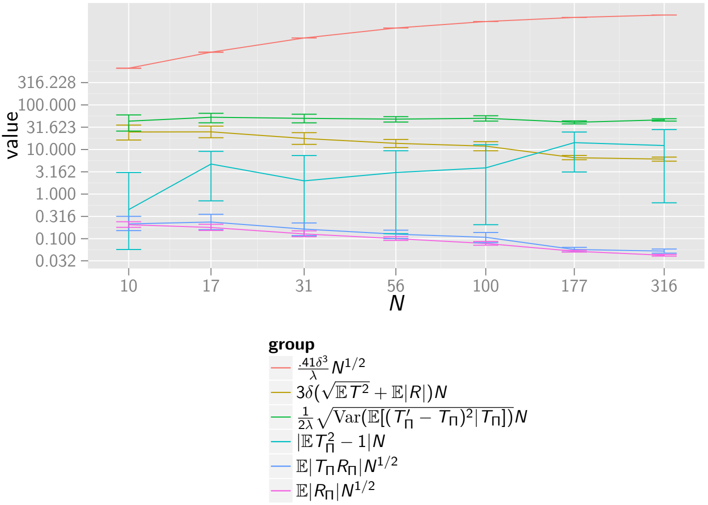

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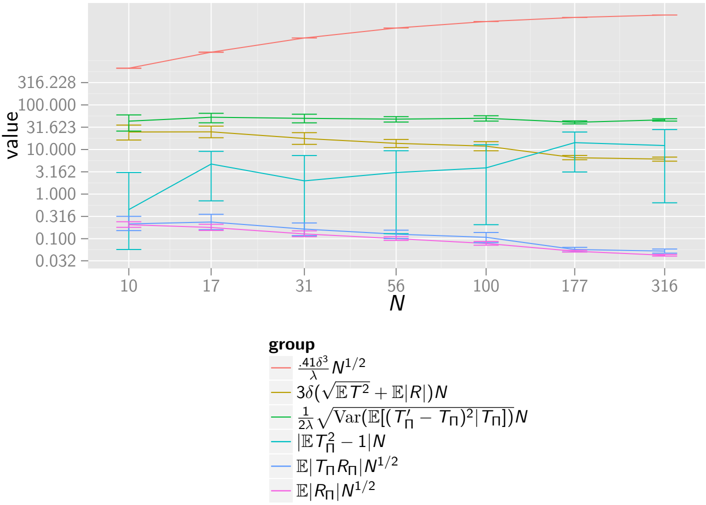
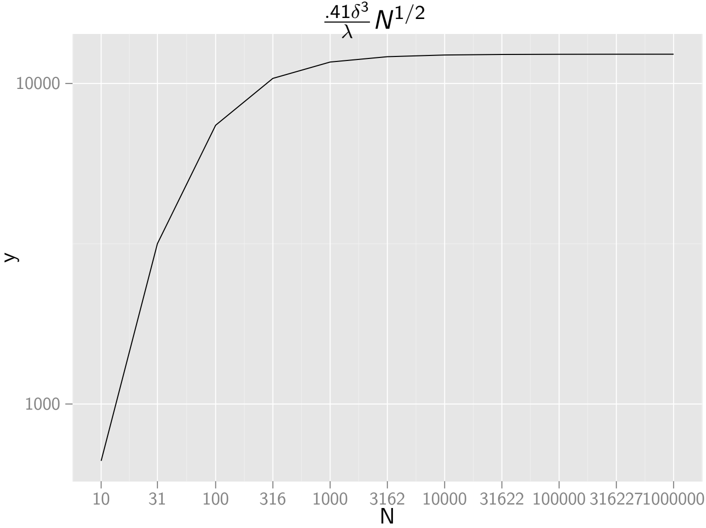
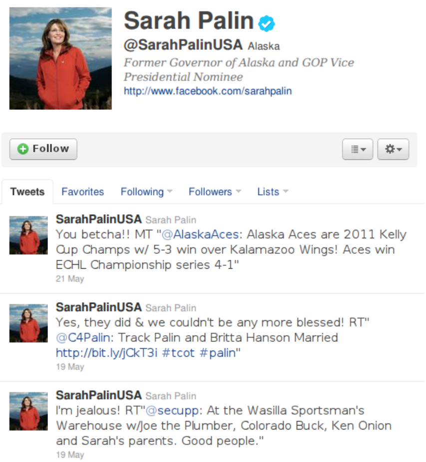


Behavior of δ



Twitter Example



Twitter Data

Raw:

```
"BarackObama: We need to reward education reforms that are
driven not by Washington, but by principals and teachers and
parents. http://OFA.BO/6p2EMy"
"SarahPalinUSA: You betcha!! MT \"@AlaskaAces: Alaska Aces
are 2011 Kelly Cup Champs w/ 5-3 win over Kalamazoo Wings!
Aces win  ECHL Championship series 4-1\""
```

After pre-processing:

```
"we need to reward education reforms that are driven not by
washington but by principals and teachers and parents "
"you betcha mt alaskaaces alaska aces are  kelly cup champs
w  win over kalamazoo wings aces win  echl championship
series "
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The Spectrum Kernel

Compares two strings based on the their length k contiguous subsequences.

- $\mathcal{X}$ is our input space, built up from an alphabet $\mathcal{A} = \{a, b, \ldots, z, \}$ with $|\mathcal{A}| = 27$.
- The k-spectrum $(k \geq 1)$ of an input sequence is the set of all length k contiguous subsequences it contains.
- Define the feature map from $\mathcal{X}$ to $\mathbb{R}^{|\mathcal{A}|^k}$ by $\Phi_k(x) = (\phi_a(x))_{a \in \mathcal{A}^k}$ where $\phi_a(x)$ is the number of times a occurs in x: $\{\#aaa, \#aab, \#aac, \ldots, \}$.
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Support Vector Machines for Regression

Consider the ℓ_1-regularized (soft-margin) support vector classification problem:

$$\begin{aligned} \underset{\mathbf{w}\in\mathcal{H}, b\in\mathbb{R}}{\text{minimize}} \quad & \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{M}\xi_i \\ \text{subject to} \quad & y_i(\mathbf{w}^t\mathbf{x}_i + b) \geq 1 - \xi_i \\ & \xi_i \geq 0 \qquad\qquad \text{for all } i = 1, \ldots, m. \end{aligned}$$

For the Friedman Test, our scoring function is the margin $f(\mathbf{x}_i) = \sum_{i=1}^{m} y_i\alpha_i k(\mathbf{x}, \mathbf{x}_i) + b$.

Twitter Example

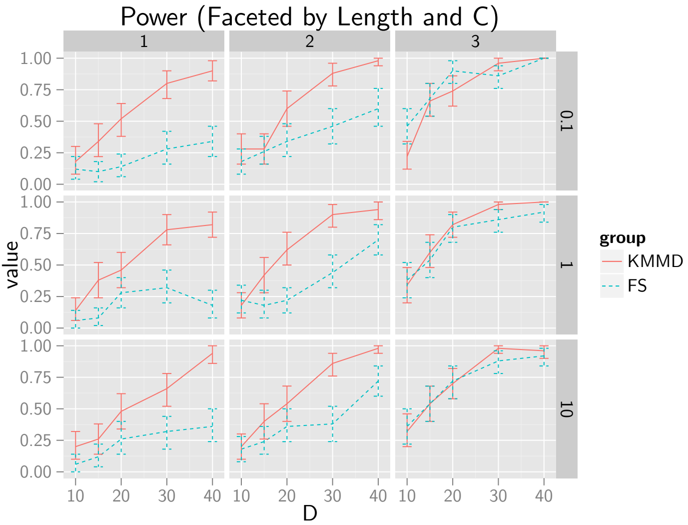


Image Data (Roosters)

Caltech 101 Object Categories [?] (297 $\times$ 300 grayscale)

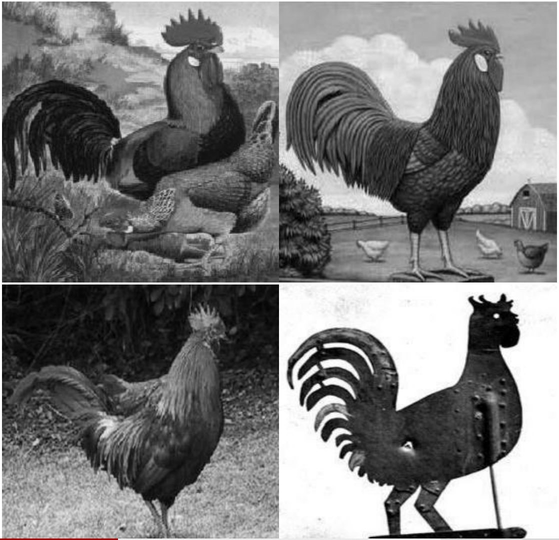
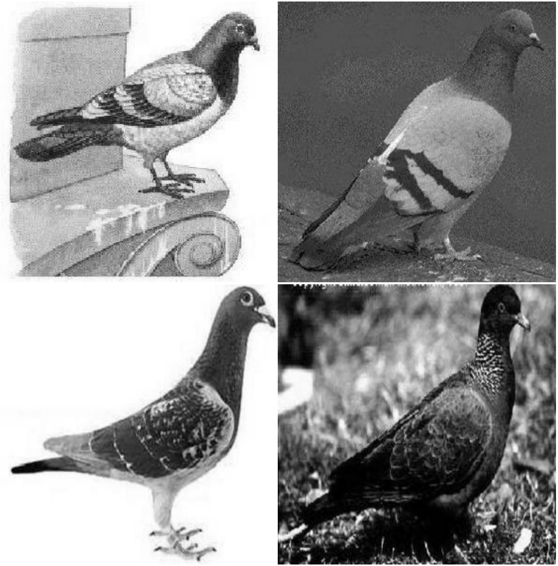


Image Data (Pigeons)



Polynomial Kernel

Each $m \times n$ grayscale image is converted to a vector of length $p = mn$.
Given $X \in \mathbb{R}^{n \times p}$, the linear kernel is given by

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

The kernel matrix is given simply by $XX^T \succeq 0$. This corresponds to the identity mapping: $\Phi(x) = x$.
The homogeneous polynomial kernel,

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

corresponds to the mapping
$\Phi(x) = [x_1^d, \ldots, x_p^d, x_1^{d-1} x_2, \ldots, x_p^{d-1} x_{p-1}]^T \in \mathbb{R}^{d'}$, where $d' = \binom{d+N-1}{d}$.

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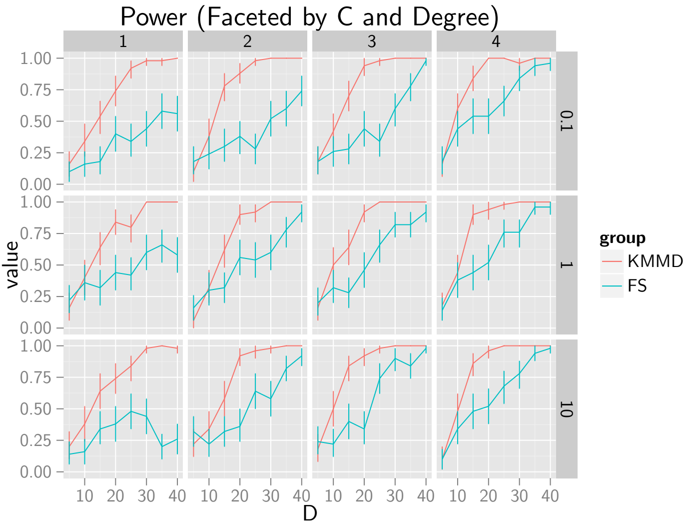
Rooster/Pigeon Example



Simulated Data

Generate independent DNA sequences of length $N \sim \text{Pois}(100)$ according to the transition matrix

$$M(p^*) = \begin{array}{c c} & \begin{array}{cccc} A & C & T & G \end{array} \\ \begin{array}{c} A \\ C \\ T \\ G \end{array} & \begin{pmatrix} \frac{1-p^*}{3} & p^* & \frac{1-p^*}{3} & \frac{1-p^*}{3} \\ \frac{1-p^*}{3} & \frac{1-p^*}{3} & p^* & \frac{1-p^*}{3} \\ \frac{1-p^*}{3} & \frac{1-p^*}{3} & \frac{1-p^*}{3} & p^* \\ p^* & \frac{1-p^*}{3} & \frac{1-p^*}{3} & \frac{1-p^*}{3} \end{pmatrix} \end{array}$$

with stationary distribution $\begin{pmatrix} .25 & .25 & .25 & .25 \end{pmatrix}$.

p takes $p^* = .25$, and q takes $p^* > .25$.

p and q generate similar numbers of 1-mers, but q can generate more AC, CT, TG, GA 2-mers.

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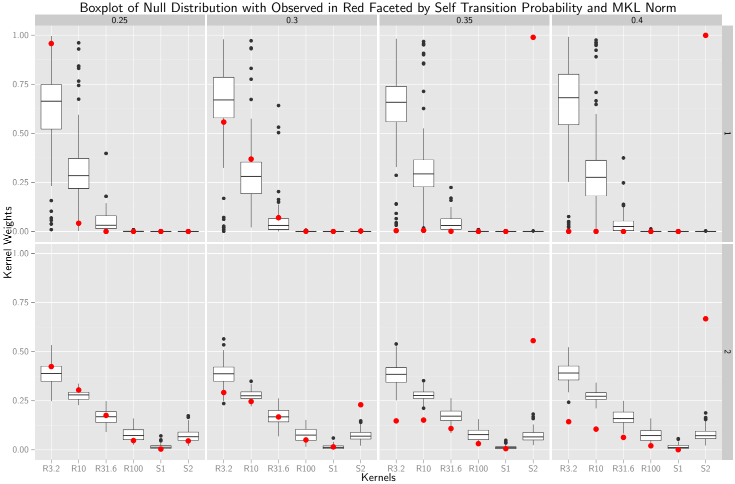
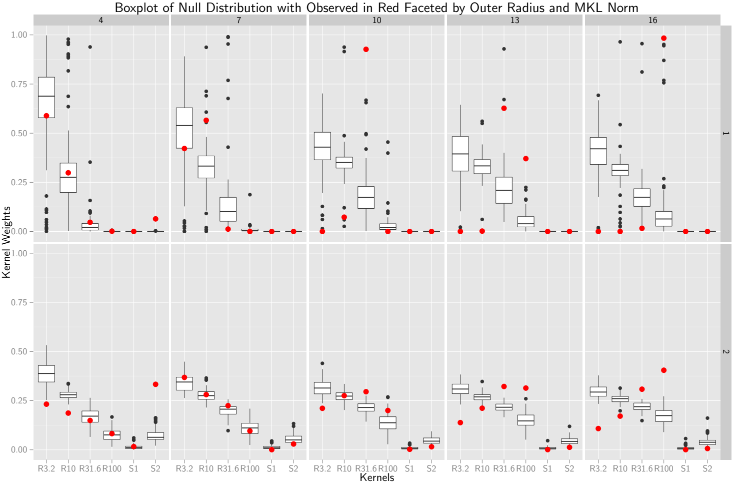
MKL

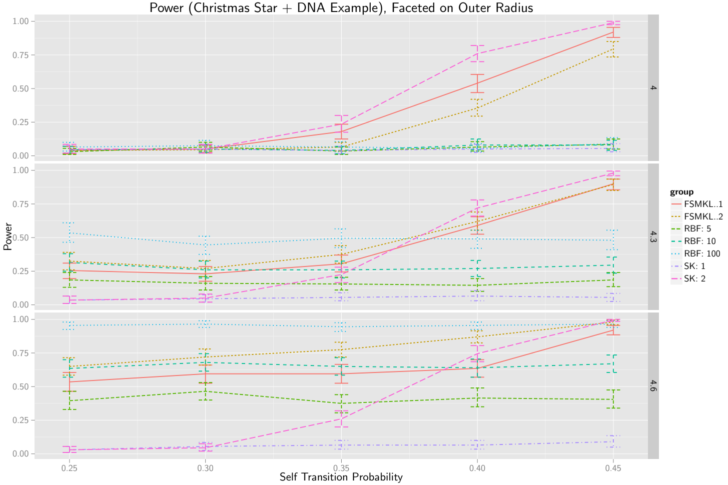

Boxplot of Null Distribution with Observed in Red Faceted by Self Transition Probability and MKL Norm
0.25
0.3
0.35
0.4
1
2
Kernel Weights
1.00
0.75
0.50
0.25
0.00
R3.2
R10
R31.6
R100
S1
S2
Kernels

MKL



Boxplot of Null Distribution with Observed in Red Faceted by Outer Radius and MKL Norm
4
7
10
13
16
1
2
Kernel Weights
1.00
0.75
0.50
0.25
0.00
R3.2
R10
R31.6
R100
S1
S2
Kernels

MKL



Power (Christmas Star + DNA Example), Faceted on Outer Radius
Power
Self Transition Probability
0.00
0.25
0.50
0.75
1.00
0.25
0.30
0.35
0.40
0.45
4
4.3
4.6
group
FSMKL..1
FSMKL..2
RBF: 5
RBF: 10
RBF: 100
SK: 1
SK: 2

Future Work

- Generalize theory for higher dimensional settings and/or non-linear scoring functions
- Develop similarities with Hotelling's T^2-test
- Explore performance on different types of data, in particular, unstructured data such as images
- Heterogeneous data: optimal combinations of kernels via SDPs, KL divergence

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