Entropy, Spanner Graphs, and Pattern Matching

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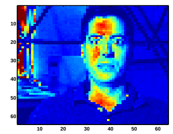
- Background: Entropic Euclidean Graphs
- Clustering applications
- Pattern matching applications
- Example: manifold learning

Image Retrieval



QUERY

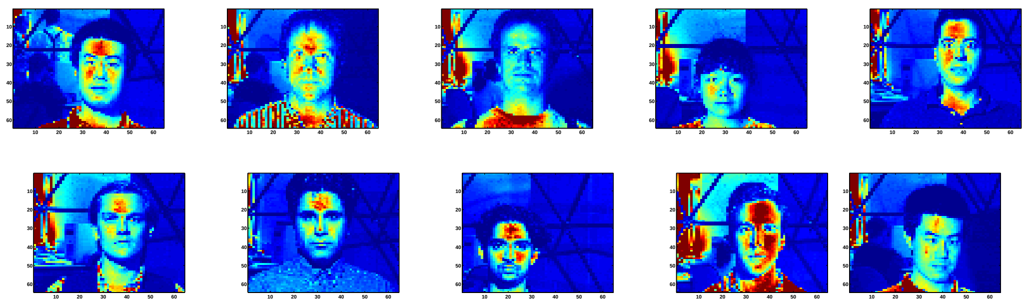
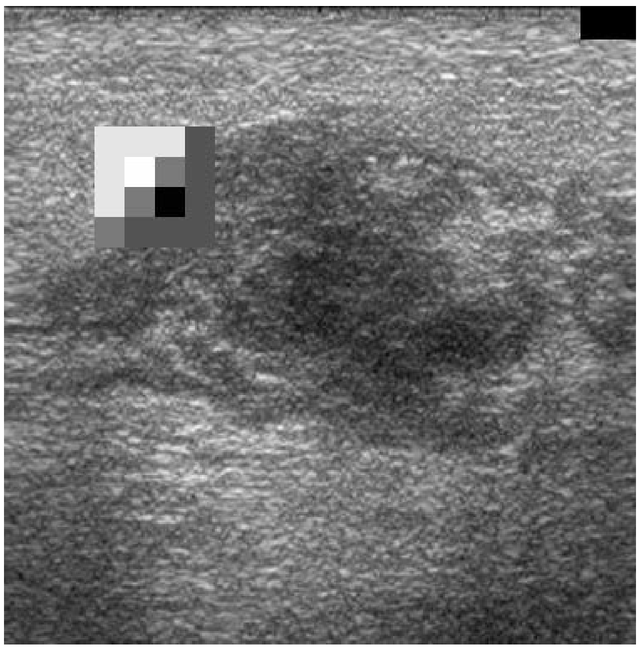


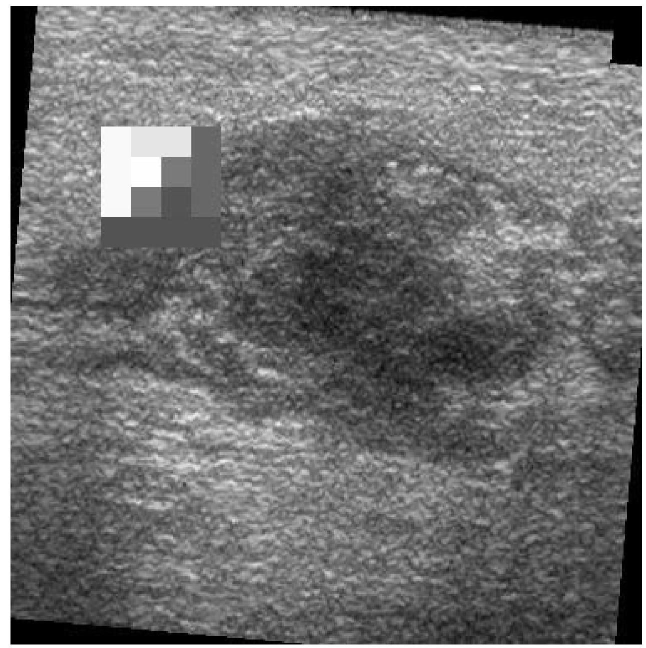
Figure 1: Yale face database `http://cvc.yale.edu/projects/yalefaces/yalefaces.html`

DATABASE

Image Registration



(a) Image I^R



(b) Image I^T

Figure 2: Local Tag Coincidences (Heemuchwala,Hero,Carson:2003)

Coincidence Scatterplot $(Z_j^R, Z_j^T)_{j=1}^p$

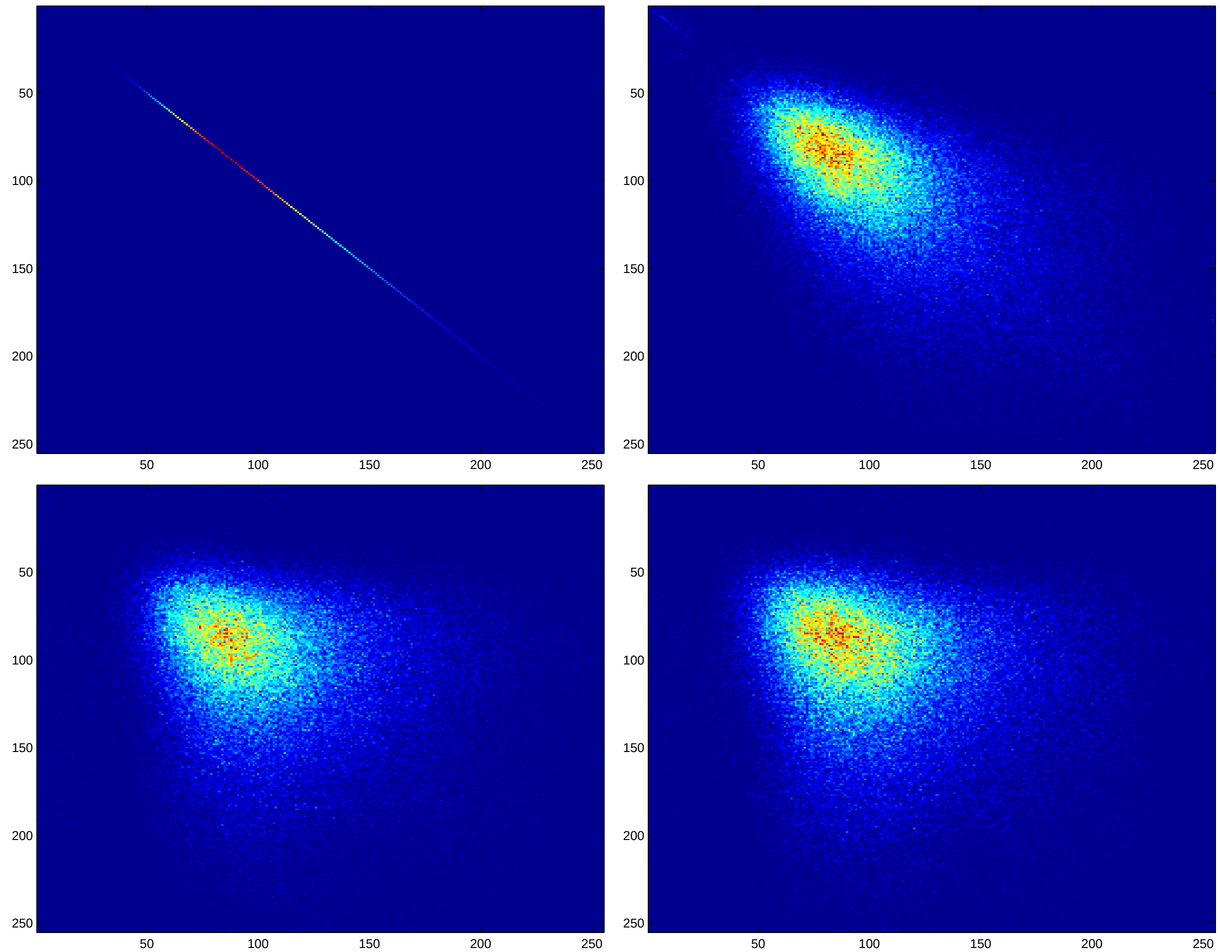
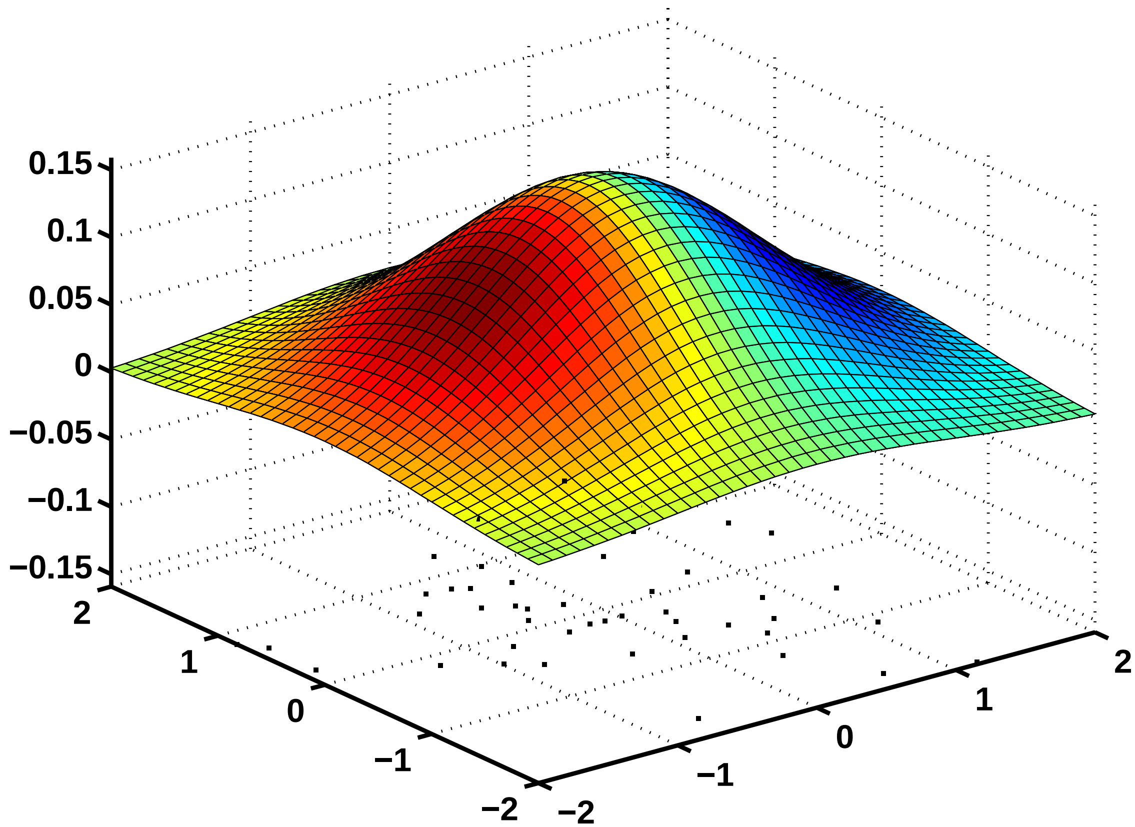


Figure 3: Grey level scatterplots. 1st Col: target=reference slice. 2nd Col: target = reference+1 slice.

High Entropy Feature Density



Basis Set for Feature Extraction

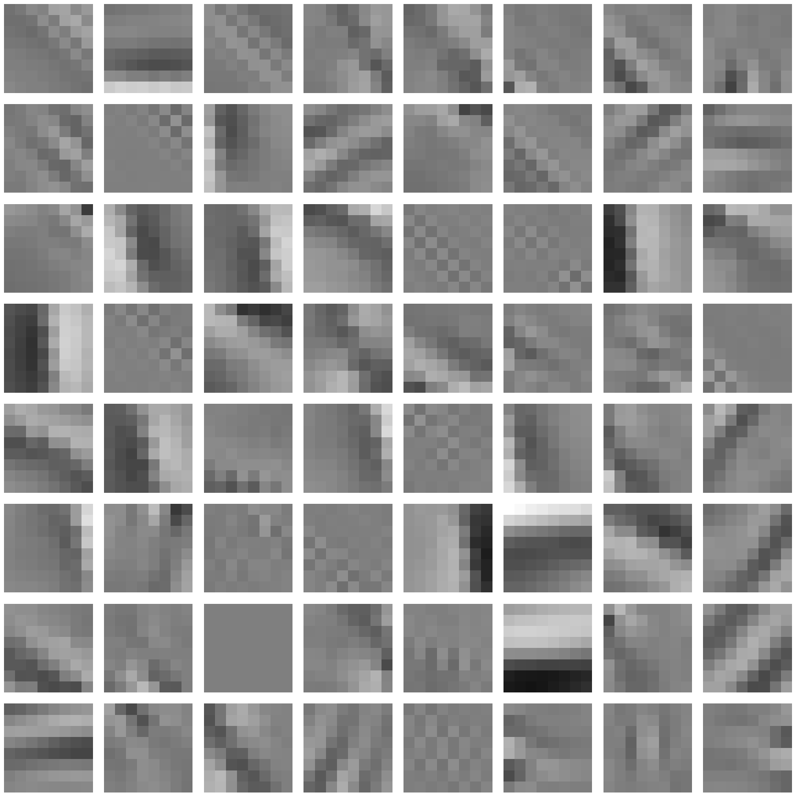


Figure 4: *ICA basis set using FastICA for breast image database*

Feature Vectors in Feature Space

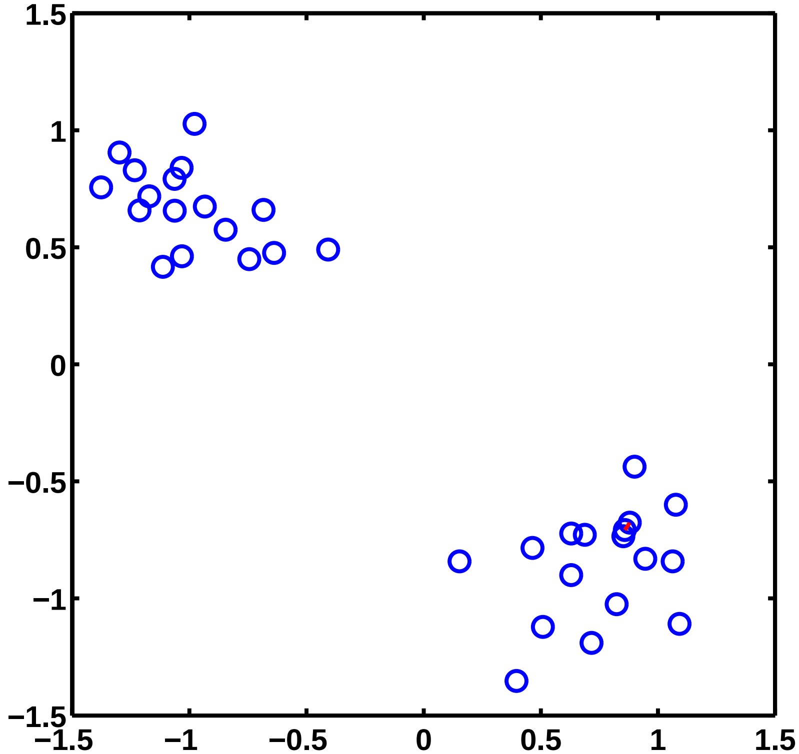
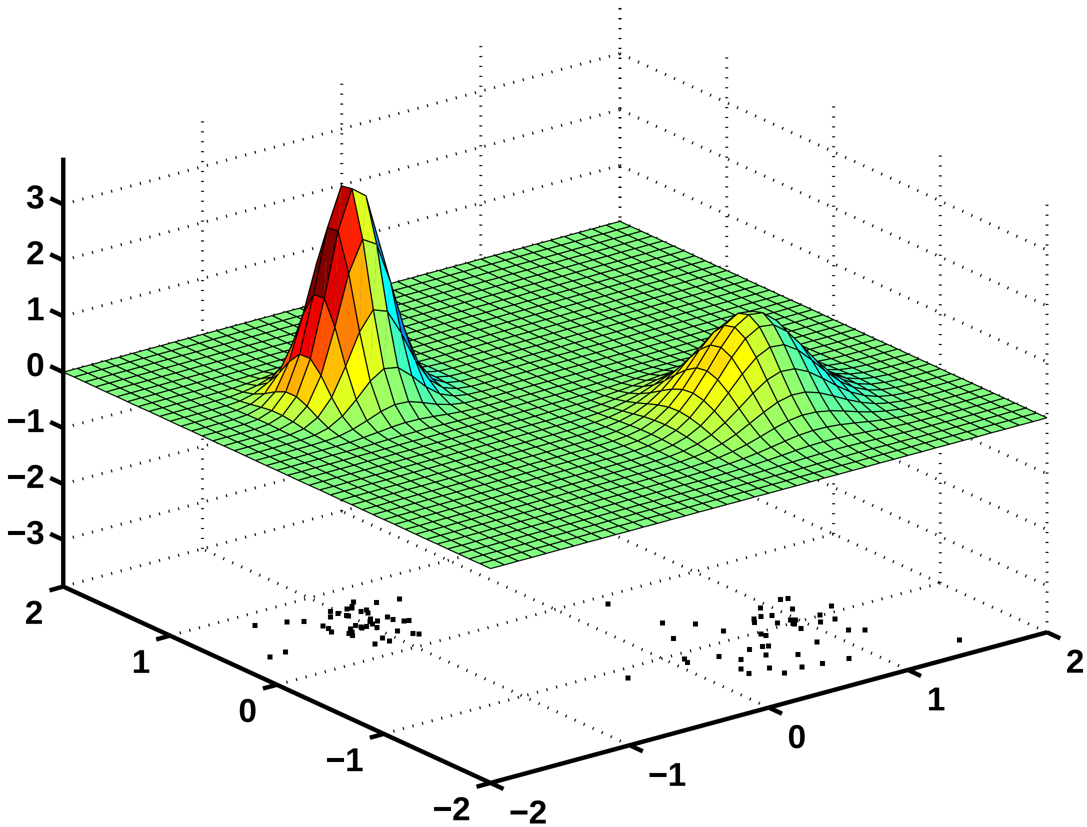
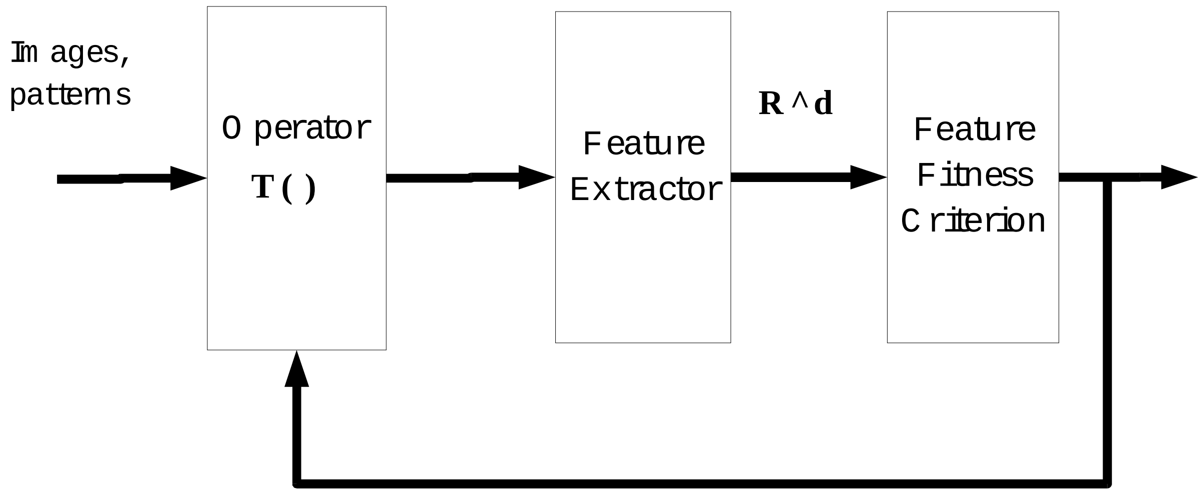


Figure 5: Vectors of projection coefficients extracted from two different images.

Feature Density over Feature Space



Common Processing System



Objective: For given fitness criterion Q, find operator T which minimizes/maximizes Q

Our focus: entropic fitness criterion $Q(f)$

f: feature density over $x \in [0,1]^d$

Some Popular Entropic Q's

1. Shannon Entropy of feature density f

$$Q(f) = H(f) = -\int f(x) \ln f(x)\, dx$$

2. Jensen difference between feature densities f, g:

$$Q(f,g) = H(\varepsilon f + (1-\varepsilon)g) - \varepsilon H(f) - (1-\varepsilon)H(g)$$

3. KL Divergence between feature densities f, g

$$Q(f,g) = D(f\|g) = \int f(x) \ln\left(\frac{f(x)}{g(x)}\right) dx$$

4. Mutual information between feature sets $f_{X,Y}$

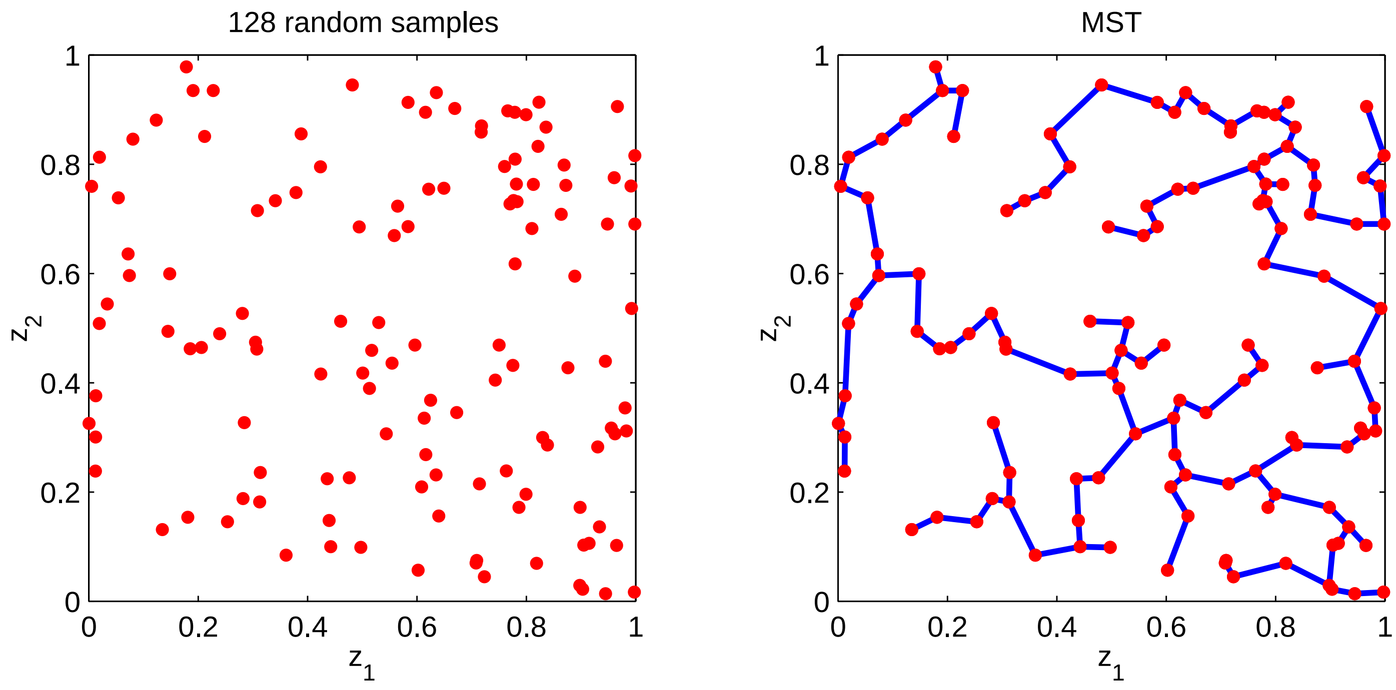
$$Q(f_{X,Y}) = \mathrm{MI}(X,Y) = \int\int f_{X,Y}(x,y) \ln\left(\frac{f_{X,Y}(x,y)}{f_X(x)\, f_Y(y)}\right) dx$$

Issue: How to estimate entropic Q from measured data?

Some possibilities:

1. Assume parameteric models for f, g, $f_{X,Y}$ (Vasconcelos&Lipman:2000,Stoica&etal:1998)
2. Substitute non-parametric density estimates of f, g, $f_{X,Y}$
   (a) Quantize feature space and use histogram estimates (Beirlant&etal:1997)
   (b) Use adaptive partitioning density estimates (Vasicek:1976, Miller:2002, Gray&etal:2000)
3. Use "entropic graphs" which emulate/estimate Q (Hero&Michel:1997,Neemwuchwala,Hero&Carson:2002)

A Set of Feature Samples and a Euclidean Spanning Graph

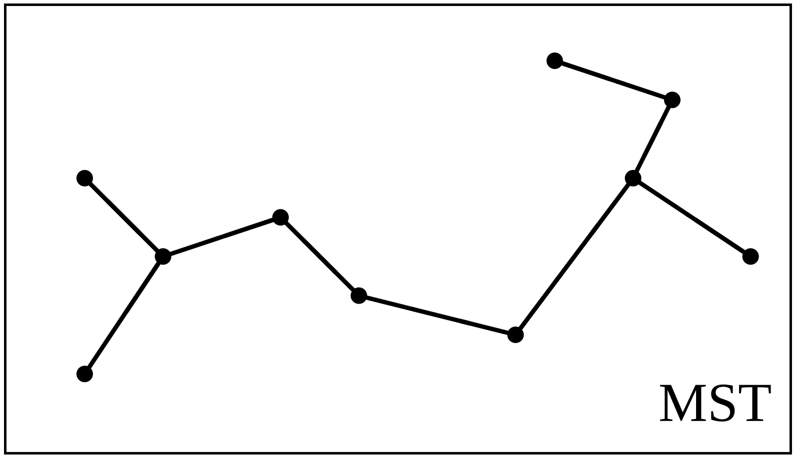


Minimal Euclidean Graphs: MST

Let $\mathrm{T}_n = \mathrm{T}(X_n)$ denote the possible sets of edges in the class of acyclic graphs spanning X_n (spanning trees).

The Euclidean Power Weighted MST achieves

$$L_\gamma^{\mathrm{MST}}(X_n) = \min_{\mathrm{T}_n} \sum_{e \in \mathrm{T}_n} \|e\|^\gamma.$$

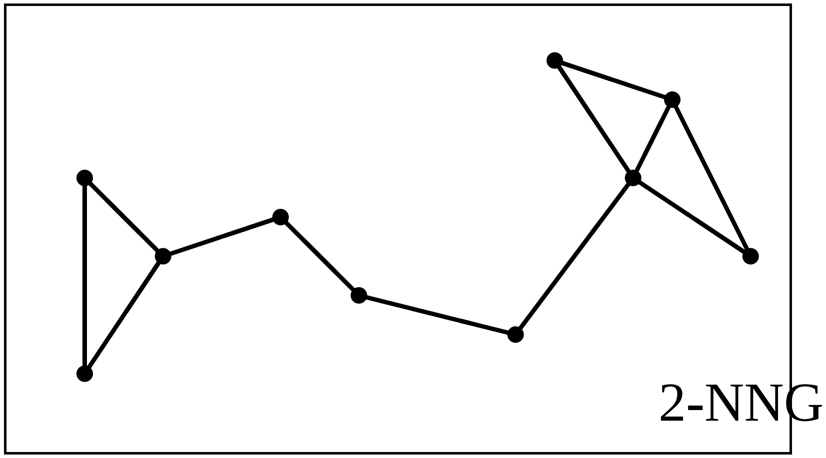


Minimal Euclidean graphs: k-NNG

Let $N_{k,i}(X_n)$ denote the possible sets of k edges connecting point x_i to all other points in X_n.

The Euclidean Power Weighted k-NNG is

$$L_\gamma^{k-NNG}(X_n) = \sum_{i=1}^{n} \min_{N_{k,i}(X_n)} \sum_{e \in N_{k,i}(X_n)} |e|^\gamma$$



MST for Two Different Samples

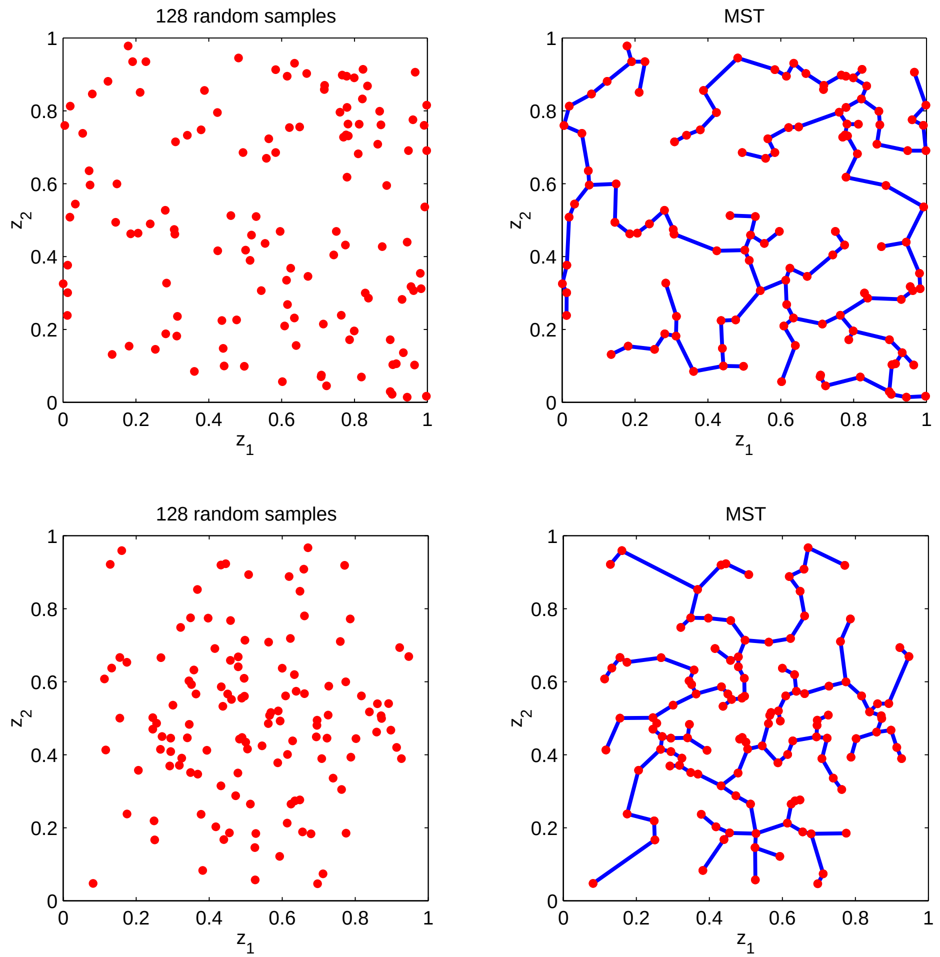


Figure 6:

Large n behavior of MST

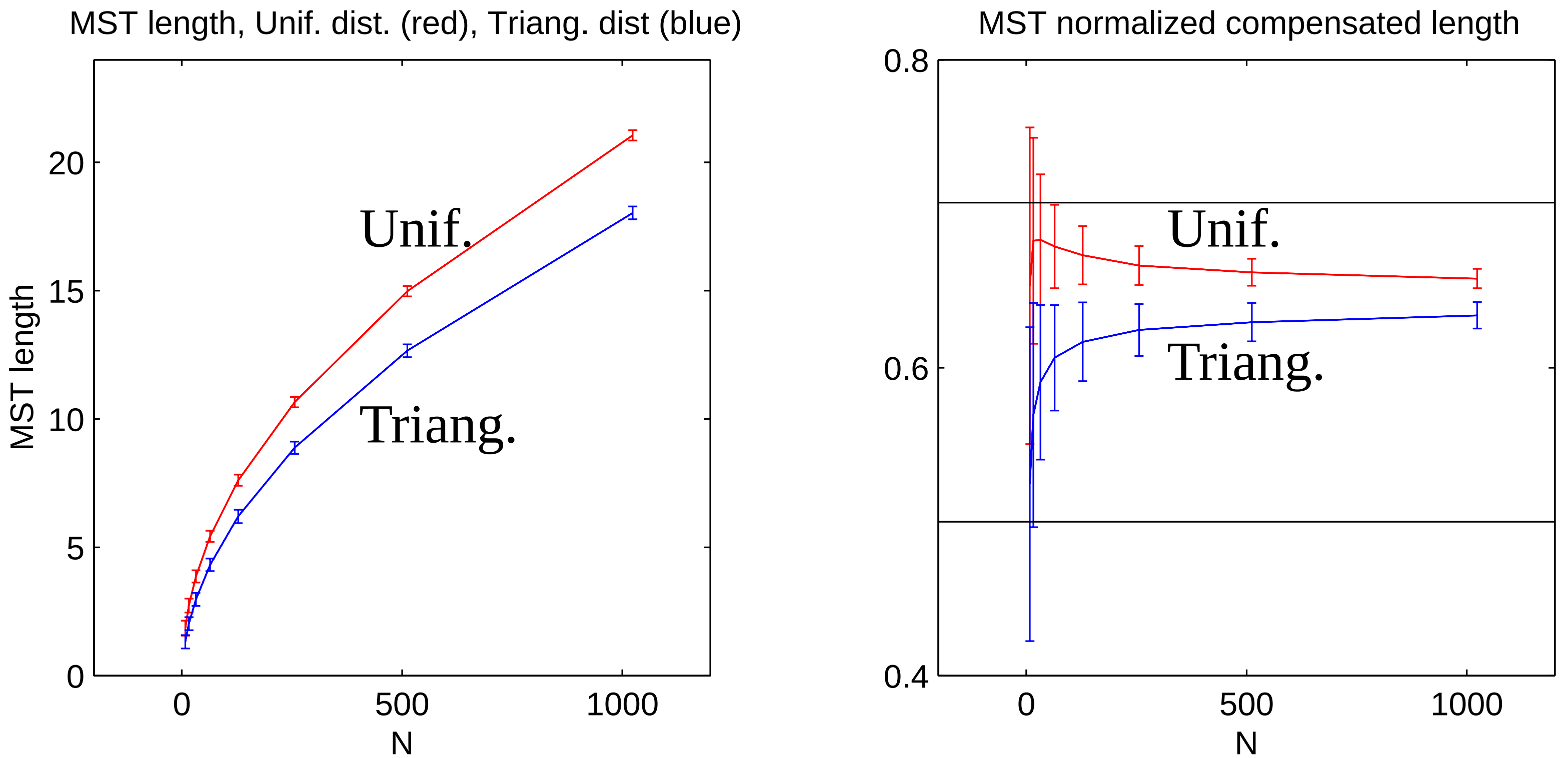


Figure: MST and log MST weights as function of the number of samples.

Asymptotics: the BHH Theorem

Define the MST length functional

$$L_\gamma(\mathcal{X}_n) = \min_{T_n} \sum_{e \in T_n} \|e\|^\gamma.$$

Theorem 1 *[Beardwood, Halton&Hammersley:1959] Let* $\mathcal{X}_n = \{X_1, \ldots, X_n\}$ *be an i.i.d. realization from a Lebesgue density* f *with support* $S \subset [0,1]^d$.

$$\lim_{n\to\infty} L_\gamma(\mathcal{X}_n)/n^{(d-\gamma)/d} \quad = \quad \beta_{L_\gamma,d} \int_S f(x)^{(d-\gamma)/d} dx, \qquad (a.s.)$$

Or, letting $\alpha = (d-\gamma)/d$

$$\frac{1}{1-\alpha} \ln\left(L_\gamma(\mathcal{X}_n)/n^\alpha\right) \quad \to \quad H_\alpha(f) + c \qquad (a.s.)$$

Rényi Entropy and Divergence

- Rényi Entropy of order α [Rényi:61,70]

$$H_\alpha(f) = \frac{1}{1-\alpha} \ln \int_S f^\alpha(x) dx$$

- Rényi α-divergence of fractional order $\alpha \in [0,1]$

$$\begin{aligned} D_\alpha(f_1 \parallel f_0) &= \frac{1}{\alpha - 1} \ln \int_S f_0 \left(\frac{f_1}{f_0}\right)^\alpha dx \\ &= \frac{1}{\alpha - 1} \ln \int_S f_1^\alpha f_0^{1-\alpha} dx \end{aligned}$$

  – α-Divergence vs. Kullback-Liebler divergence

$$\lim_{\alpha \to 1} D_\alpha(f_1 \| f_0) = \int f_1 \ln \frac{f_1}{f_0} dx.$$

α-Divergence and Decision Theoretic Error Exponents

Let Z_i be i.i.d.:

$$\begin{aligned} H_0 &: \quad Z_i \sim f \\ H_1 &: \quad Z_i \sim g \end{aligned}$$

Bayes probability of error

$$P_e(n) \quad = \quad \beta(n)P(H_1) + \alpha(n)P(H_0)$$

Sanov bound (Blahut:1987,Dembo&Zeitouni:98)

$$\begin{aligned} \liminf_{n\to\infty} \frac{1}{n} \log P_F(n) &= -\sup_{\alpha\in[0,1]} \{(1-\alpha)D_\alpha(g\|f)\} \\ \liminf_{n\to\infty} \frac{1}{n} \log P_M(n) &= -\sup_{\alpha\in[0,1]} \{(1-\alpha)D_\alpha(f\|g)\}. \end{aligned}$$

Extension of BHH to Divergence Estimation?

Question: How to generalize entropic graph estimates of

$$\frac{1}{1-\alpha}\ln\int f^{\alpha}(x)dx \quad \textbf{to} \quad \frac{1}{\alpha-1}\ln\int f^{\alpha}(x)g^{1-\alpha}(x)dx \ ?$$

One possibility:

- $g(x)$: a **known** reference density on $[0,1]^d$
- Assume $f \ll g$, i.e. for all x such that $g(x)=0$ we have $f(x)=0$.
- Make measure transformation $M(x)$ such that $dx \to g(x)dx$ on $[0,1]^d$. Then for $Y_n = M(X_n)$

$$L_\gamma(Y_n)/n^{\alpha} \quad \to \quad \beta_{L_\gamma,d}\int\left(\frac{f(x)}{g(x)}\right)^{\alpha} g(x)dx, \qquad (a.s.)$$

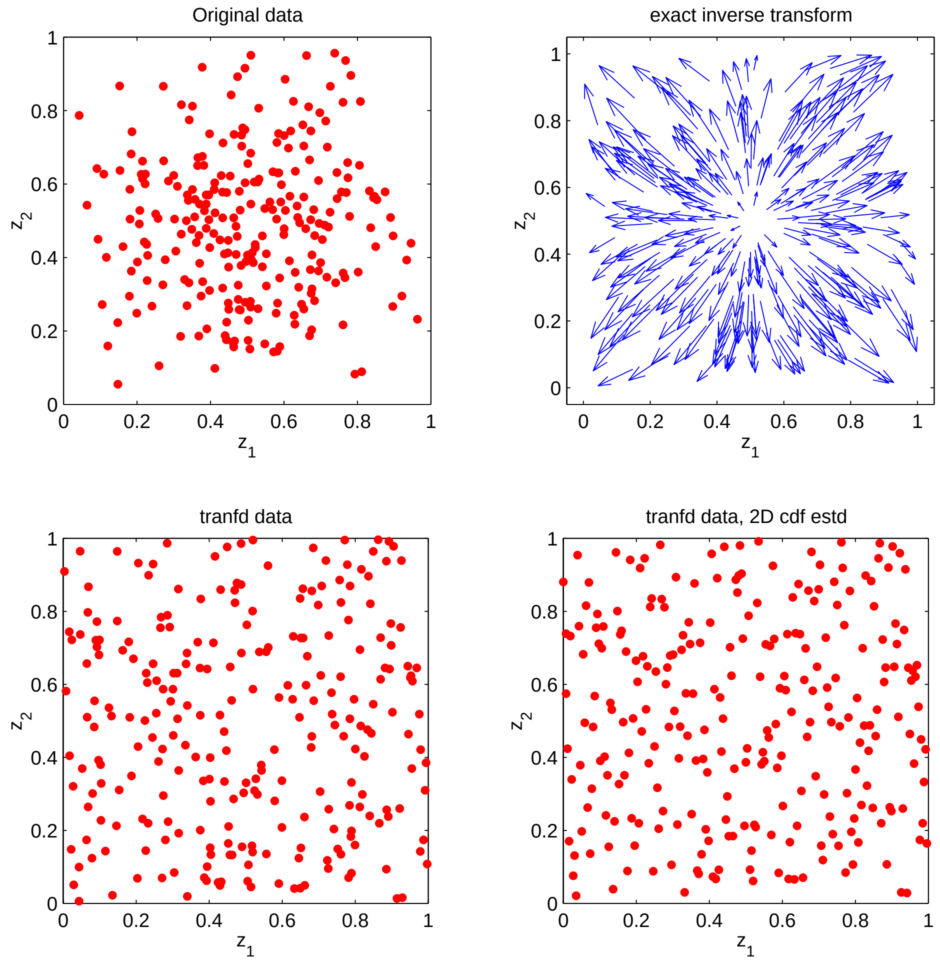


Figure 7: Top Left: i.i.d. sample from triangular distribution, Top Right: exact transformation, Bottom: after application of exact and empirical transformations.

Entropic Graphs for Clustering and Outlier Rejection: k-MST

Assume f is a mixture density of the form

$$f = (1-\varepsilon) f_1 + \varepsilon f_o,$$

where

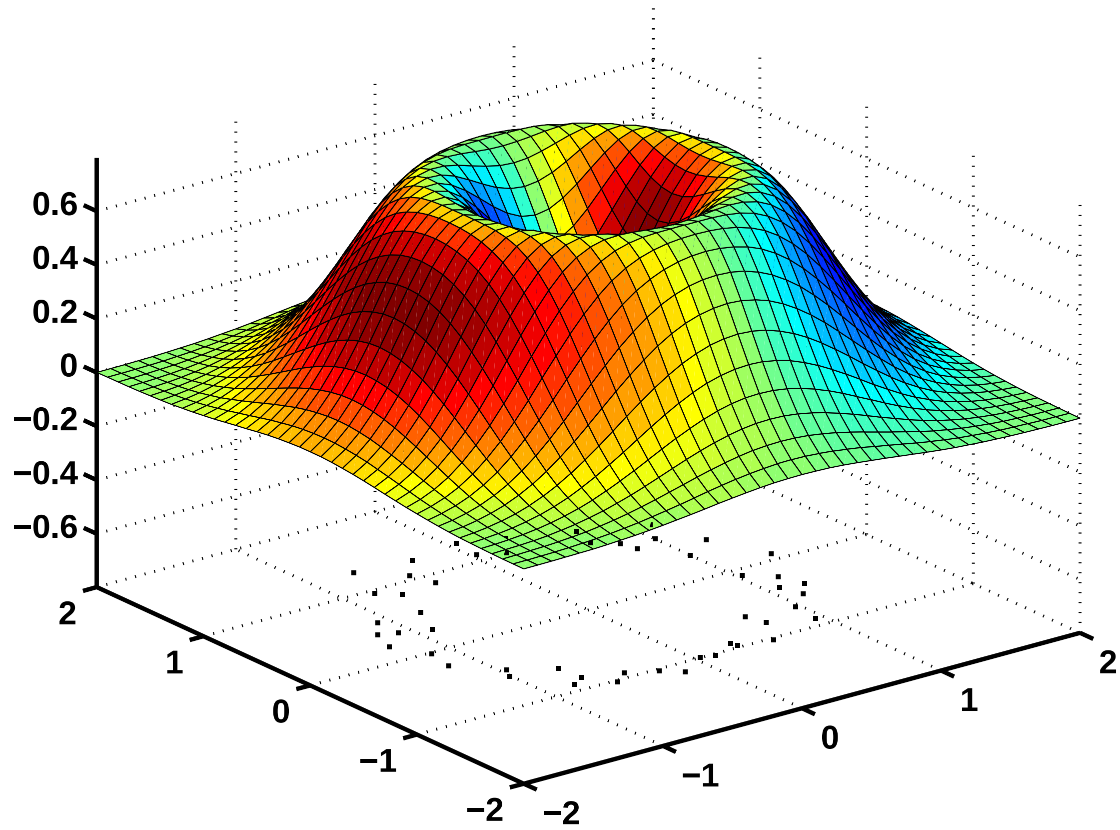
- f_o is a known ”outlier” density
- f_1 is an unknown target density
- $\varepsilon \in [0,1]$ is unknown mixture parameter

Objective: given realization X_n from f cluster the realizations from f_1.

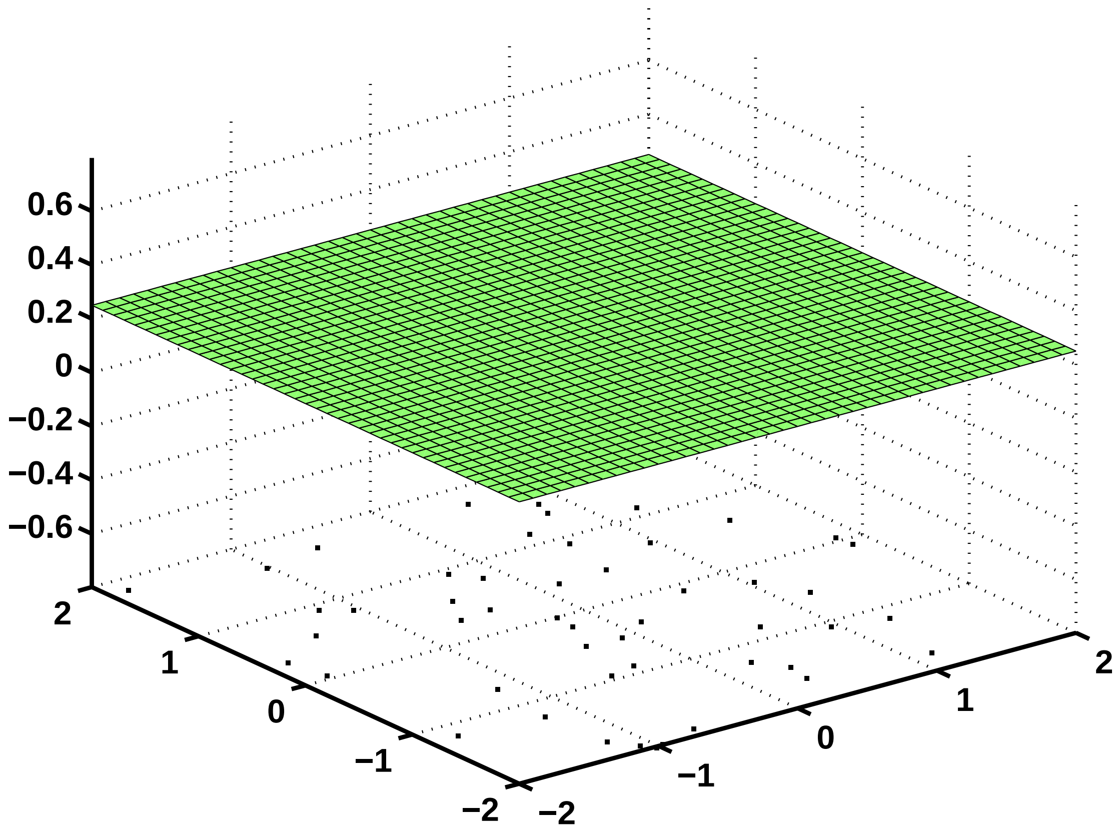
Two-step k-MST procedure:

1. Convert f_o to maxent (uniform) density via measure transformation
2. ”Prune” the MST on transformed X_n to eliminate vertices arising from maxent density

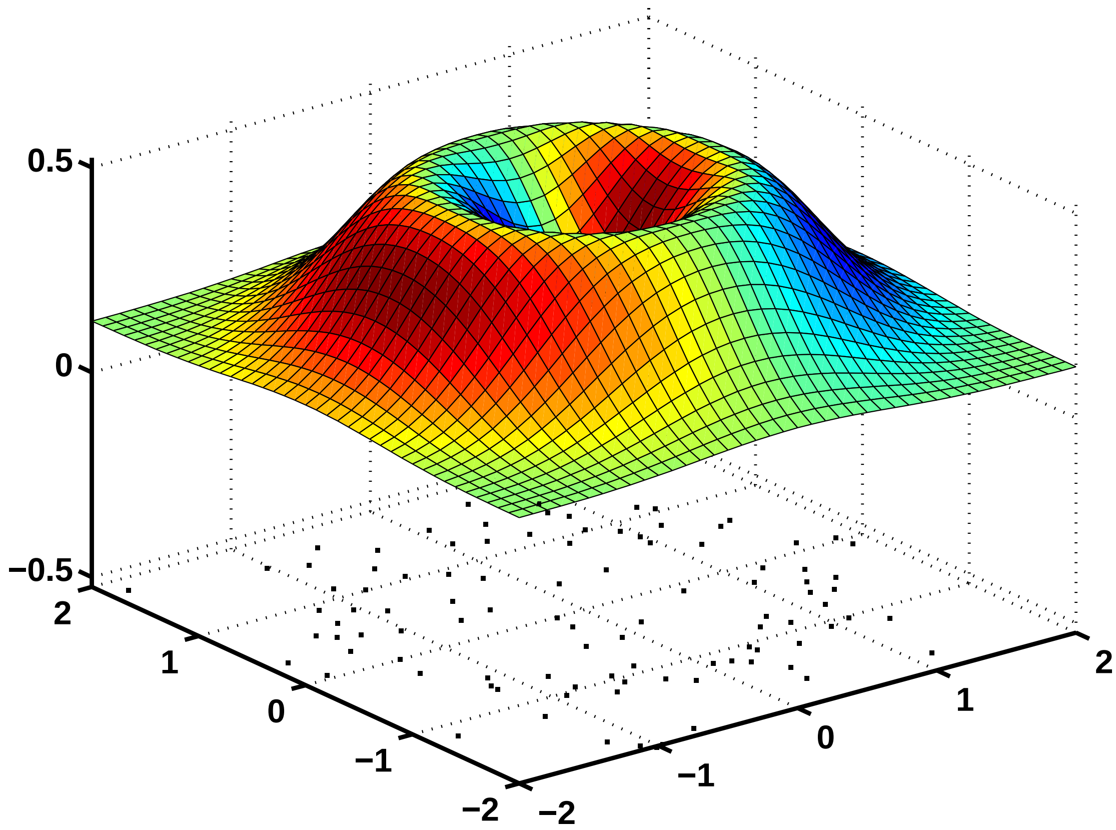
Example: Annulus Target Density f_1



Uniform Outlier Density f_o



Mixture Density



k-point Minimal Spanning Tree (*k*-MST)

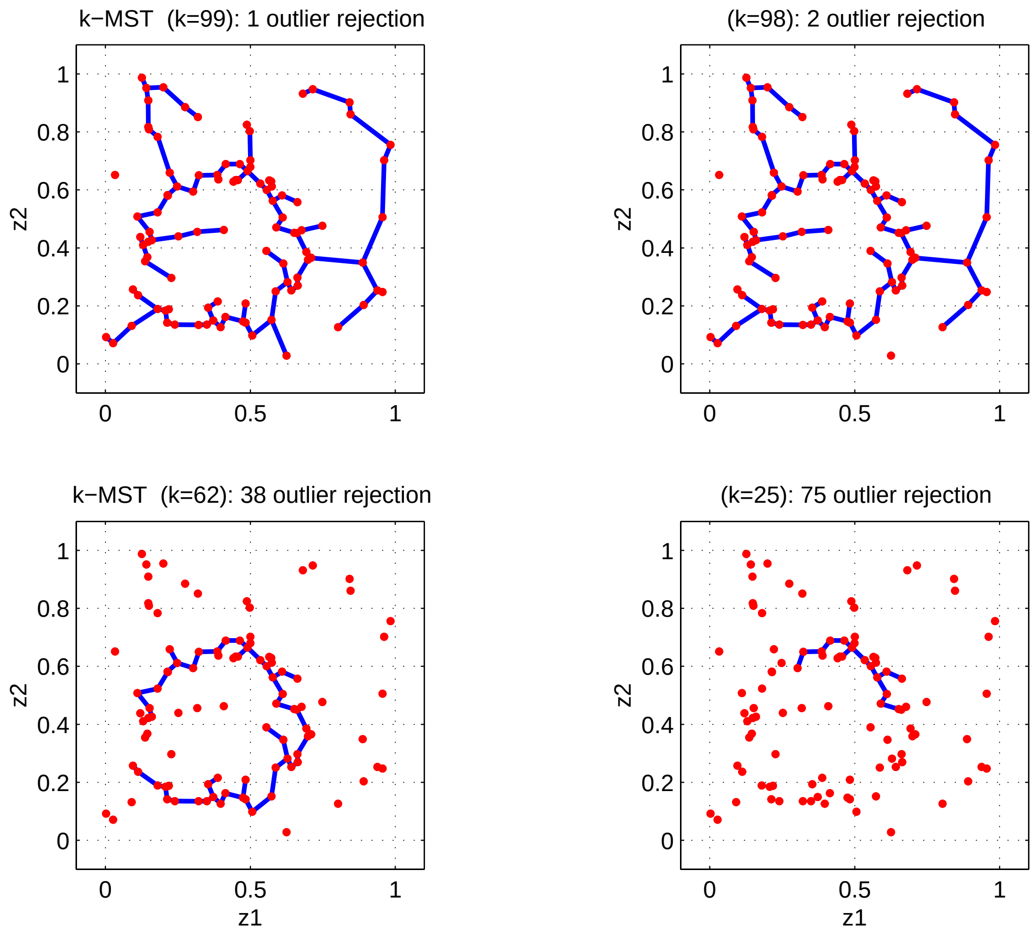


Figure 8: *Clustering an annulus density from uniform noise via k-MST.*

k-MST Stopping Rule (Hero&Michel:1997)

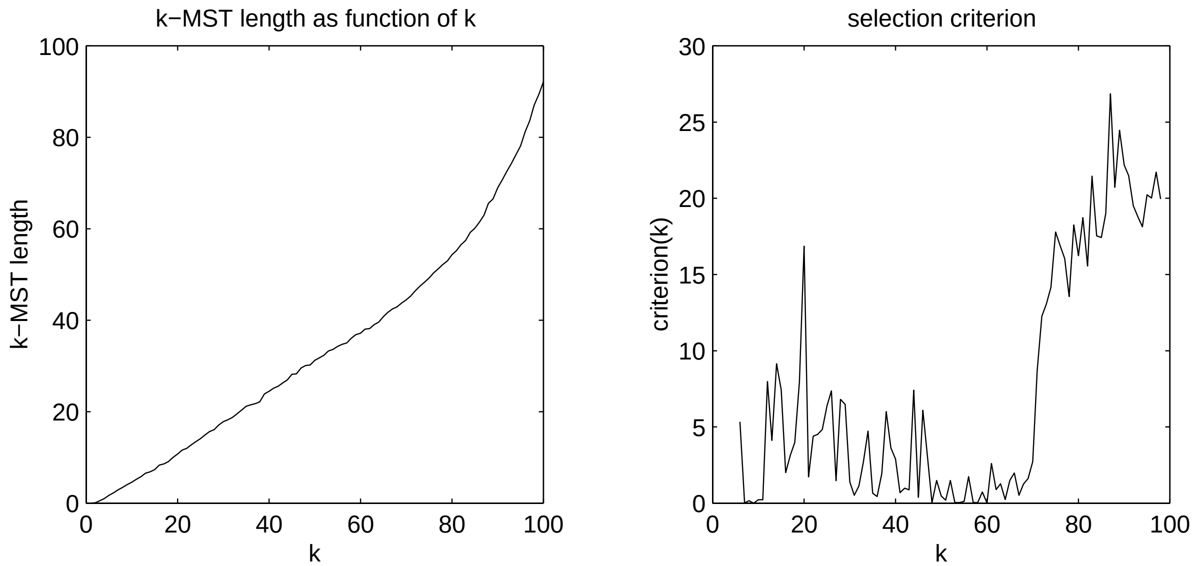


Figure 9: *Left: k-MST curve for 2D annulus density with addition of uniform "outliers" has a knee in the vicinity of $n-k=35$.*

Greedy partioning approximation to k-MST (Ravi&etal:1996)

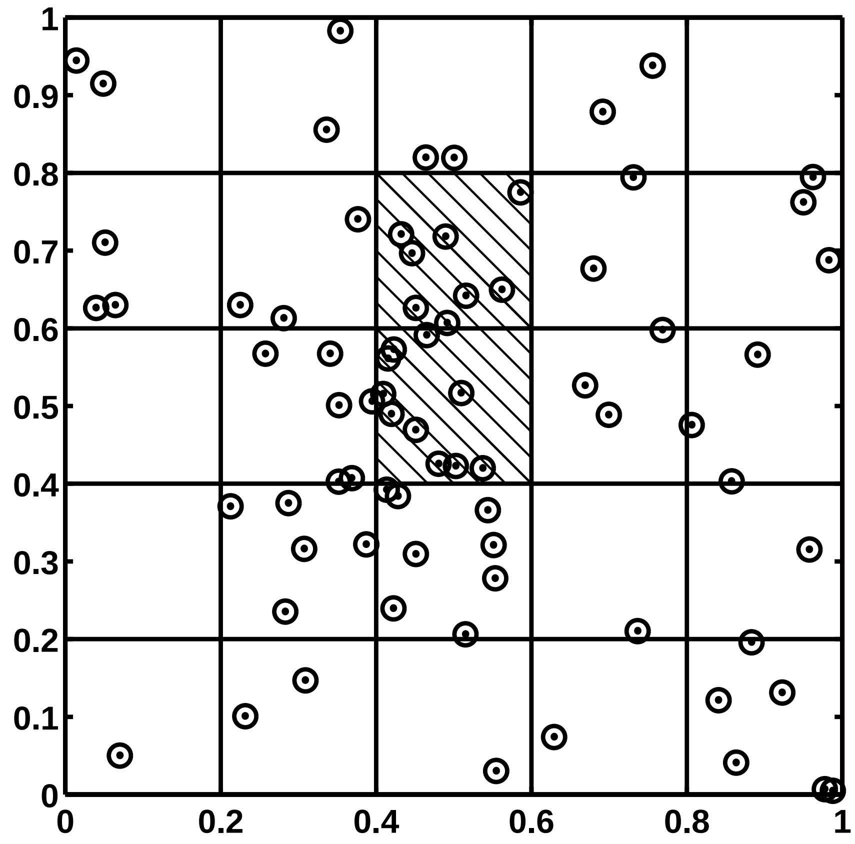


Figure 10: *A smallest subset B_k^m is the union of the two cross hatched cells shown for the case of $m = 5$ and $k = 17$.*

Extended BHH Theorem for Greedy k-MST (Hero&Michel:1999)

Fix $\rho \in [0,1]$. If $k/n \to \rho$ then the length of the greedy partitioning k-MST satisfies [Hero&Michel:IT99]

$$L_\gamma(X^*_{n,k})/(\lfloor \rho n \rfloor)^\alpha \to \beta_{L_\gamma,d} \int_S f^\alpha(x|x \in A_o)dx \qquad (a.s.)$$

where A_o is level set of f which satisfies $\int_{A_o} f = \rho$. Alternatively, with

$$H_\alpha(f|x \in A_o) = \frac{1}{1-\alpha} \ln \int_S f^\alpha(x|x \in A_o)dx$$

$$\frac{1}{1-\alpha} \ln \left(L_\gamma(X^*_{n,k})/(\lfloor \rho n \rfloor)^\alpha\right) \to \beta_{L_\gamma,d} H_\alpha(f|x \in A_o) + c \qquad (a.s.)$$

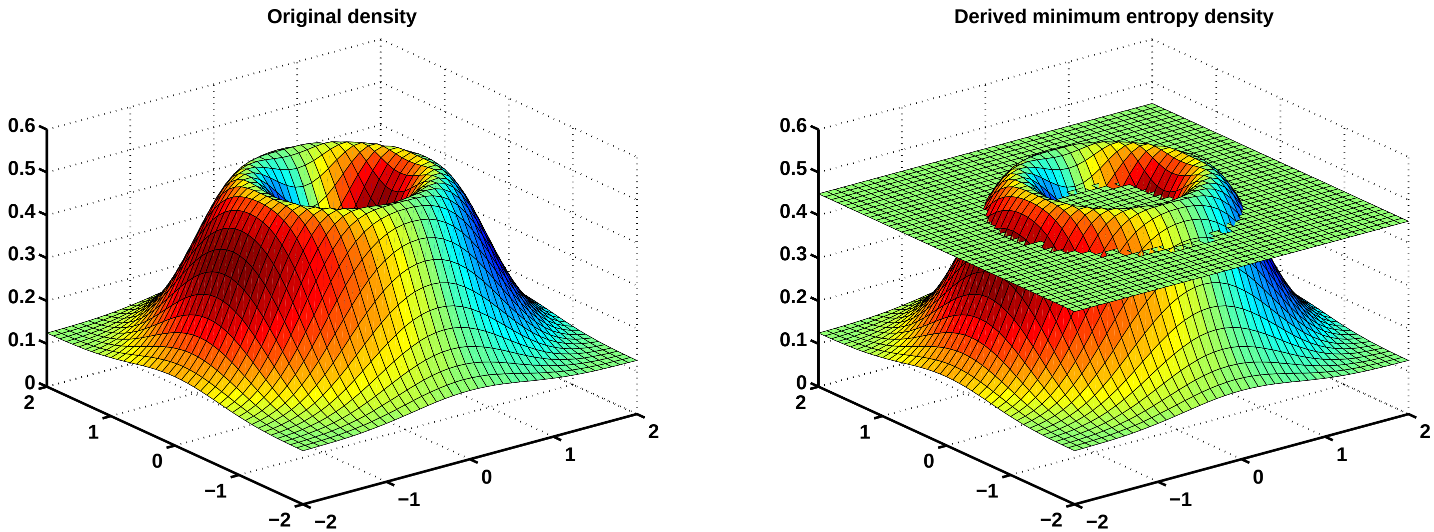


Figure 11: Waterpouring contruction of minimum entropy density.

k-MST Influence Function

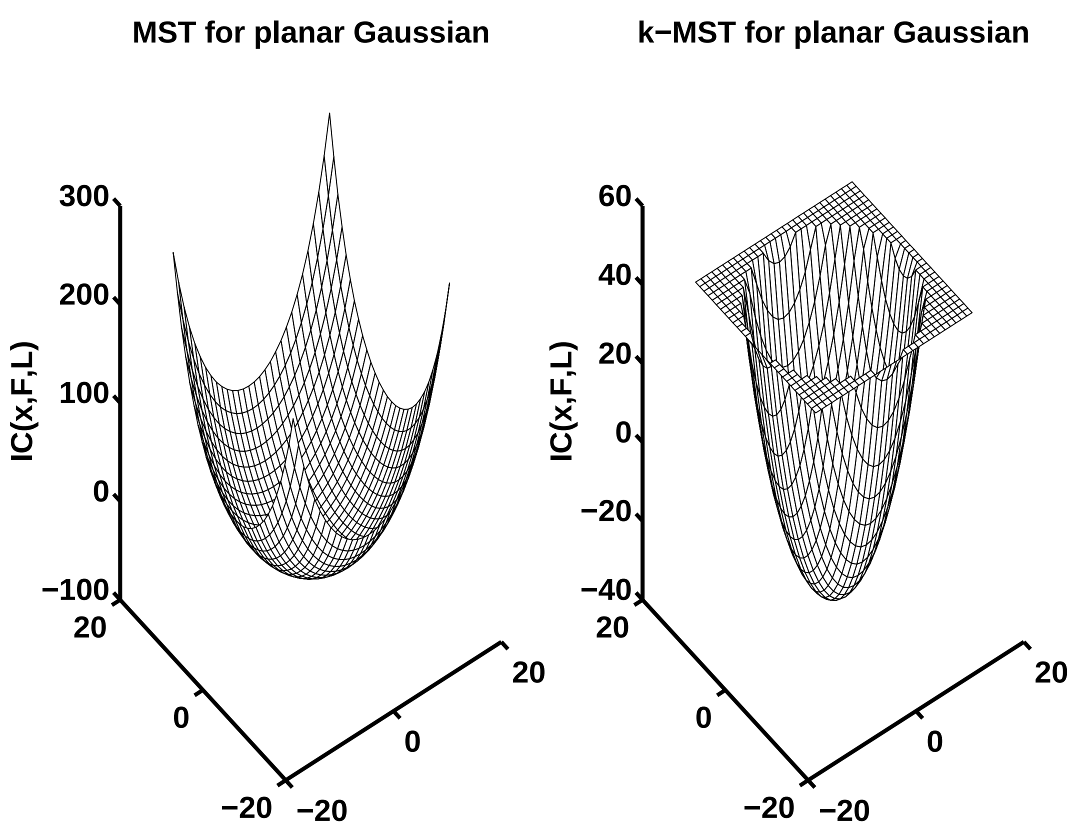


Figure 12: *MST and k-MST influence curves for Gaussian density on the plane.*

What is the entropic graph's convergence rate?

Theorem 2 (Hero,Costa&Ma:2001) *Let $d \geq 2$ and $1 \leq \gamma \leq d-1$. Assume $X_1, \ldots, X_n$ are i.i.d. random vectors over $[0,1]^d$ with density $f \in \Sigma_d(\beta, l)$, $\beta, l > 0$, having support $S \subset [0,1]^d$. Assume also that $f^{\frac{1}{2}-\frac{\gamma}{d}}$ is integrable. Then,*

$$O\left(n^{-r_1(d,\beta)}\right) \leq \sup_{f \in \Sigma_d(\beta,l)} E\left[\left|L_\gamma(X_1,\ldots,X_n)/n^{(d-\gamma)/d} - \beta_{L_\gamma,d}\int_S f^{(d-\gamma)/d}(x)\mathrm{d}x\right|^p\right]^{1/p} \leq O\left(n^{-r_2(d,\beta)}\right),$$

where

$$r_1(d,\beta) = \min\{\frac{4\beta}{4\beta+d}, 1/2\} \quad r_2(d,\beta) = \frac{\alpha\beta}{\alpha\beta+1}\,\frac{1}{d}$$

and $\alpha = \frac{d-\gamma}{d}$.

Extension to Partition Approximations

$$L_{\gamma}^{m}(X_n) = \sum_{i=1}^{m^d} L_{\gamma}(X_n \cap Q_i) + b(m),$$

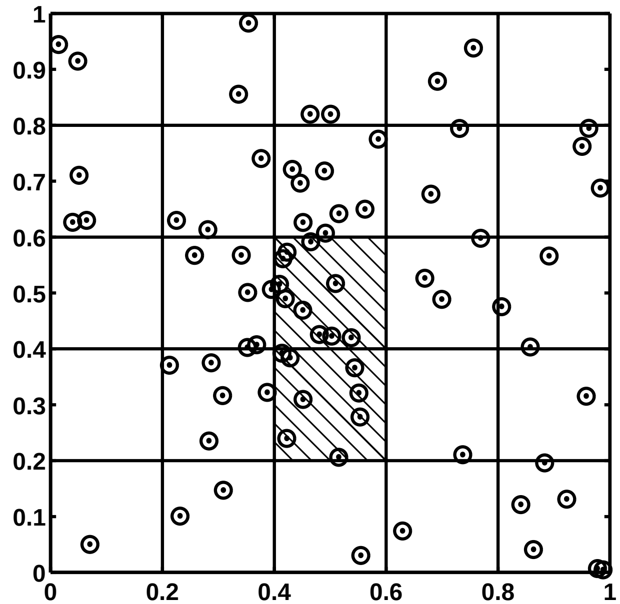


Figure 13: *Partition approximation.*

Theorem 3 (Hero,Costa&Ma:2001) *Let* $L_\gamma^m(X_n)$ *be a partition approximation to* $L_\gamma(X_n)$*. Under the same hypotheses as in the previous proposition, if* $b(m) = O(m^{d-\gamma})$

$$O\left(n^{-r_1(d,\beta)}\right) \quad \leq$$

$$\sup_{f\in\Sigma_d(\beta,l)} E\left[\left|L_\gamma^{m(n)}(X_1,\ldots,X_n)/n^{(d-\gamma)/d} - \beta_{L_\gamma,d}\int_S f^{(d-\gamma)/d}(x)\mathrm{d}x\right|^p\right]^{1/p}$$

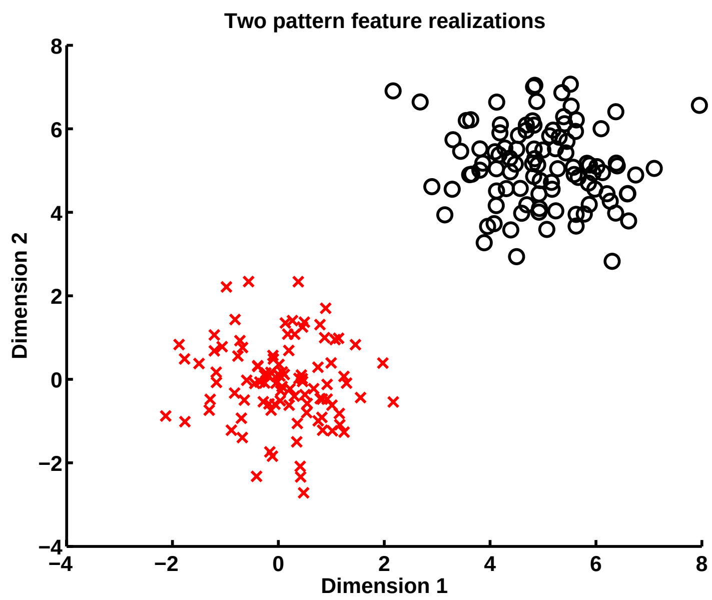
$$\leq O\left(n^{-r_3(d,\beta)}\right),$$

where

$$r_3(d,\beta) = \frac{\alpha\beta}{\frac{d-1}{\gamma}\ \alpha\beta + 1}\ \frac{1}{d}\ .$$

This bound is attained by choosing the progressive-resolution sequence $m = m(n) = n^{1/[d(\frac{d-1}{\gamma}\ \alpha\beta+1)]}$.

Entropic Graphs for Pattern Matching



Two groups of i.i.d. feature realizations on $[0,1]^d$:

- $X_m = \{X_1, \ldots, X_m\}$, $X_i \sim f$
- $Y_n = \{Y_1, \ldots, Y_n\}$, $Y_i \sim g$
- $p = m/(m+n)$, $q = 1-p$

Objective: estimate separation of f and g using X_m and Y_n

Some entropic graph estimation possibilities

Option 1. construct MST/k-NNG on pooled data $X_m \cup Y_n$ (Hero,Ma,Michel&Gorman:2001):

$$\ln L_\gamma(X_m \cup Y_n)/N^\alpha \rightarrow (1-\alpha)H_\alpha(pf+qg)+c, \quad (a.s.)$$

If subsequently subtract $\ln L(X_m)/N^\alpha$ and $\ln L(Y_n)/N^\alpha$ obtain estimator of α-Jensen difference (Basseville:1989,He&etal:2001)

$$\Delta(f,g) = H_\alpha(pf+qg) - pH_\alpha(f) - qH_\alpha(g)$$

Option 2: prune all single-class connections from pooled MST and compute normalized length

$$L_\gamma(X_m \Delta Y_n) = \frac{1}{N^\alpha}\sum_{e_{xy}} |e_{xy}|^\gamma$$

- for $\gamma = 0$ obtain ”Multivariate runs statistic” Friedman&Rafsky:1979 (FR).
- for $0 < \gamma < d$ obtain generalized FR statistic (Costa&Hero:2003)
- FR($\gamma = 0$) statistic converges a.s. to affinity (Henze&Penrose:1998)

$$A_{FR}(f,g) = 2pq \int \frac{f(x)g(x)}{pf(x)+qg(x)} dx$$

This affinity is related to divergence measure:

$$D_{FR}(f\|g) = 1 - A_{FR}(f,g) = \int \frac{p^2 f^2(x) + q^2 g^2(x)}{pf(x)+qg(x)} dx$$

Option 3: implement entropic graph approximation of adaptive partition estimators of different divergence functionals (example below).

Illustration: Jensen Difference estimator

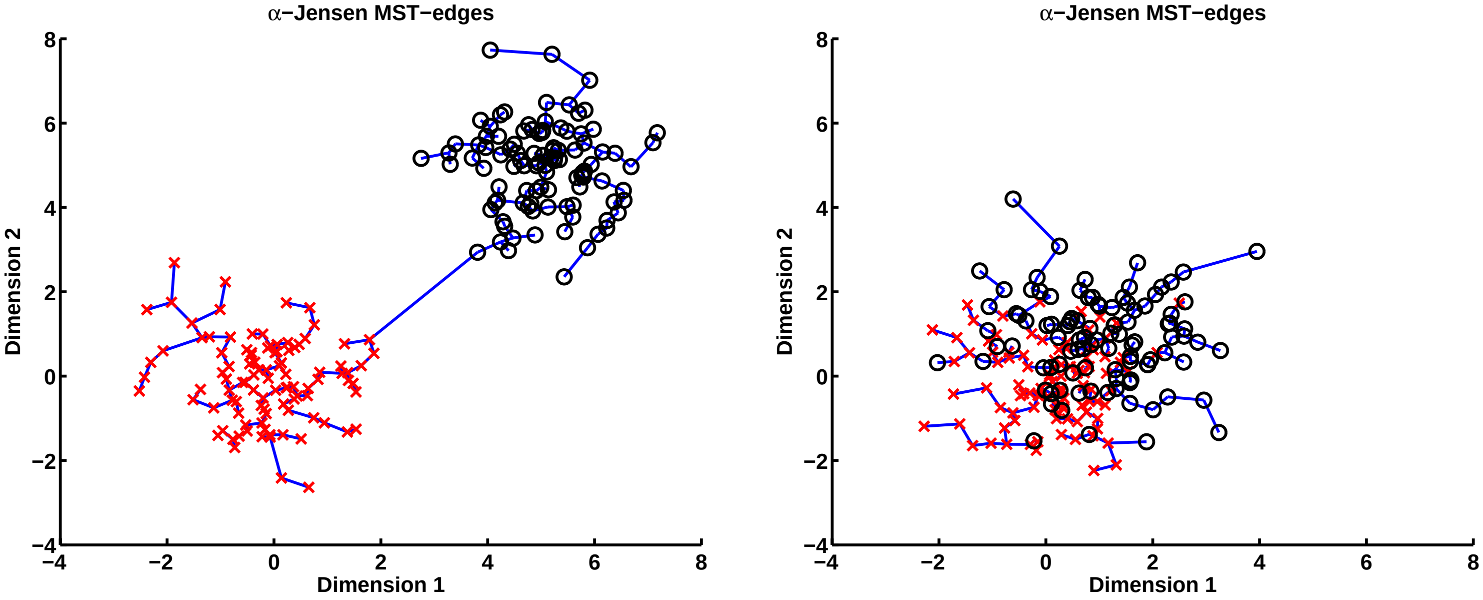
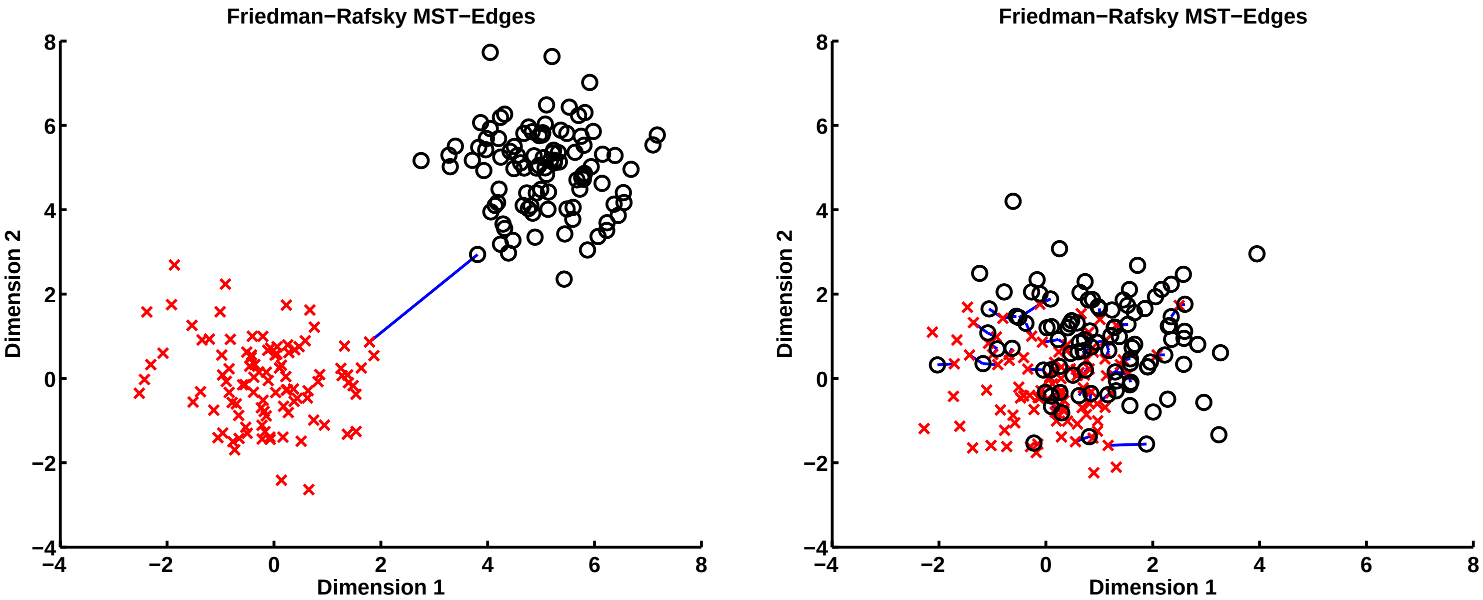


Illustration: Friedman-Rafsky Statistic



Entropic Graphs vs Adaptive-Partition Density Plug-in Estimates

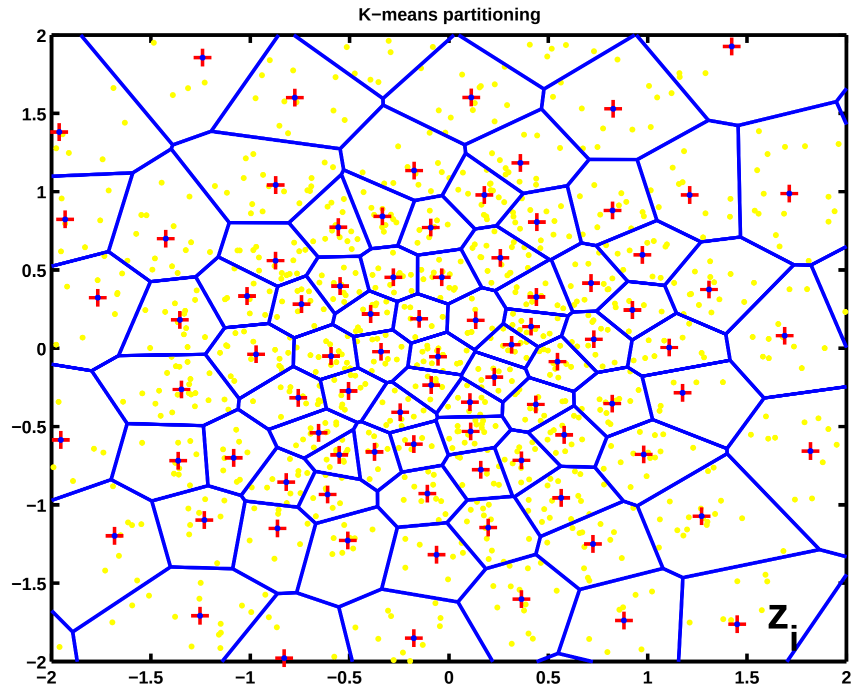
Define

$$I(f) = \int_S f^{\alpha}(x)dx$$

For N i.i.d. realizations $\{x_i\}_{i=1}^N$ from f define:

1. Π: an M-cell partition of $[0,1]^d$.
2. $\Pi(x)$: the cell in Π containing point $x \in [0,1]^d$
3. $\hat{f}_{\Pi}$: a partition estimator of f

$$\hat{f}_{\Pi}(x) = \frac{\mu(\Pi(x))}{\lambda(\Pi(x))}, \quad x \in [0,1]^d$$



For $\{z_i\}_{i=1}^N$ an i.i.d. realization **independent** of $\{x_i\}_{i=1}^N$ consider the α-entropy estimator

$$\hat{I}_\Pi \quad = \quad \frac{1}{N}\sum_{i=1}^N \hat{f}_\Pi^{\alpha-1}(z_i) = \frac{1}{N}\sum_{i=1}^N \left(\frac{\mu(\Pi(z_i))}{\lambda(\Pi(z_i))}\right)^{\alpha-1}$$

Under weak conditions on Π (Lugosi&Nobel:1996), this estimator converges a.s. to

$$E[f^{\alpha-1}(z_i)] = \int_S f^{\alpha}(x)dx = I(f)$$

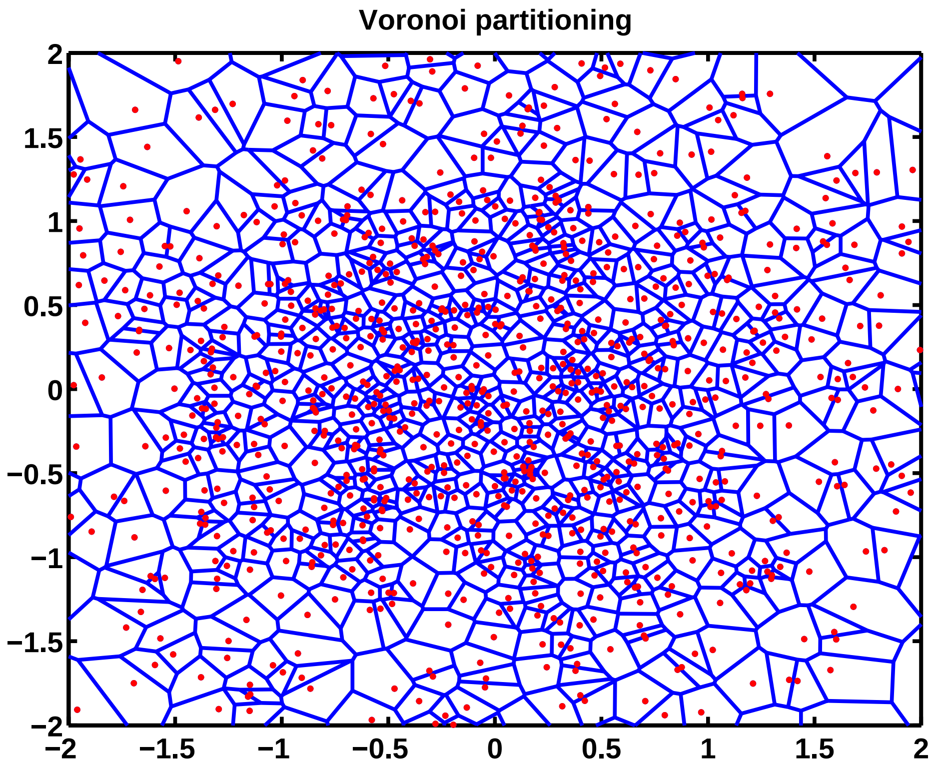
as $N \longrightarrow \infty$. Equivalently,

$$\beta_{L_\gamma,d}\hat{I}_\Pi \longrightarrow \beta_{L_\gamma,d}\int_S f^{\alpha}(x)dx$$

which corresponds to the a.s. limit of $L_\gamma(X_N)/N^{\alpha}$.

To exploit this correspondence, (formally) specialize to:

1. $\alpha = (d-\gamma)/d$
2. Π is Voronoi partition ($\mu(\Pi(x)) \equiv 1$)
3. $z_i = x_i$, $i = 1, \ldots, N$



In this case we have:

$$\beta_{L_\gamma,d}\hat{I}_\Pi = \frac{\beta_{L_\gamma,d}}{N}\sum_i \left(\frac{1}{\lambda(\Pi(z_i))}\right)^{\alpha-1} \quad = \quad \frac{\beta_{L_\gamma,d}}{N}\sum_i \left(\lambda^{1/d}(\Pi(z_i))\right)^{\gamma}$$

Q. What relation between $\lambda^{1/d}(\Pi(z_i))$ and e_i would make $\beta_{L_\gamma,d}\hat{I}_\Pi$ equal to $L_\gamma(X_N)/N^\alpha$?

A. When

$$\frac{\beta_{L_\gamma,d}}{N}\sum_i\left(\lambda^{1/d}(\Pi(z_i))\right)^\gamma \quad = \quad \frac{1}{N^\alpha}\sum_i e_i^\gamma$$

which occurs if we identify

$$\lambda^{1/d}(\Pi(z_i)) = \frac{n^{1/d}}{\beta_{L_\gamma,d}^{1/\gamma}}\, e_i \tag{1}$$

Heuristic: can use formal relation (1) to obtain entropic graph implementations of divergence estimators.

Example: Geometric-Arithmetic (GA) Affinity (Taneja:2001)

$$A(f,g) \quad = \quad \int (pf(x)+qg(x))^{\alpha} \left(f^p(x)g^q(x)\right)^{1-\alpha} dx$$

1. Pooled sample $Z_{m+n} = X_m \cup Y_m$ has density $h = pf + qg$
2. Adaptive-partition plug-in estimator of $A(f,g)$ is

$$\hat{A}_{ap} = \frac{1}{N}\sum_{z_i=1}^{N}\left(\frac{\hat{f}^p(z_i)\hat{g}^q(z_i)}{\hat{h}(z_i)}\right)^{1-\alpha} \rightarrow A(f,g) \quad (a.s.)$$

3. Specialize partition to Voronoi and substitute (1):

$$\hat{A}_{eg} = \frac{1}{N}\underbrace{\sum_i \min\left\{\left(\frac{e_i(Y_n)}{e_i(X_m)}\right)^{p\gamma}, \left(\frac{e_i(X_m)}{e_i(Y_n)}\right)^{q\gamma}\right\}}_{R_\gamma(X_m \cup Y_n)}$$

Planar Pattern Matching Simulation

- X_m realization from $N_2(\underline{0}, \mathbf{I})$
- Y_n realization from $N_2(\underline{D}, \mathbf{I})$
- Four pattern separation measures Δ investigated

$$\Delta = \begin{array}{cc} L_\gamma(X_m \cup Y_n)/N^\alpha, & L_0(X_m \Delta Y_n)/N \\ L_\gamma(X_m \Delta Y_n)/N^\alpha, & R_\gamma(X_m \cup Y_n)/N \end{array}$$

- $\gamma = 1$, $\alpha = 1/2$
- Local resolution measure

$$\rho(\Delta) = \frac{|E[\Delta|D=0] - E[\Delta|D=1]|}{\sqrt{\sigma_\Delta^2(D=0) + \sigma_\Delta^2(D=1)}}$$

Pattern Matching Simulation: Convergence

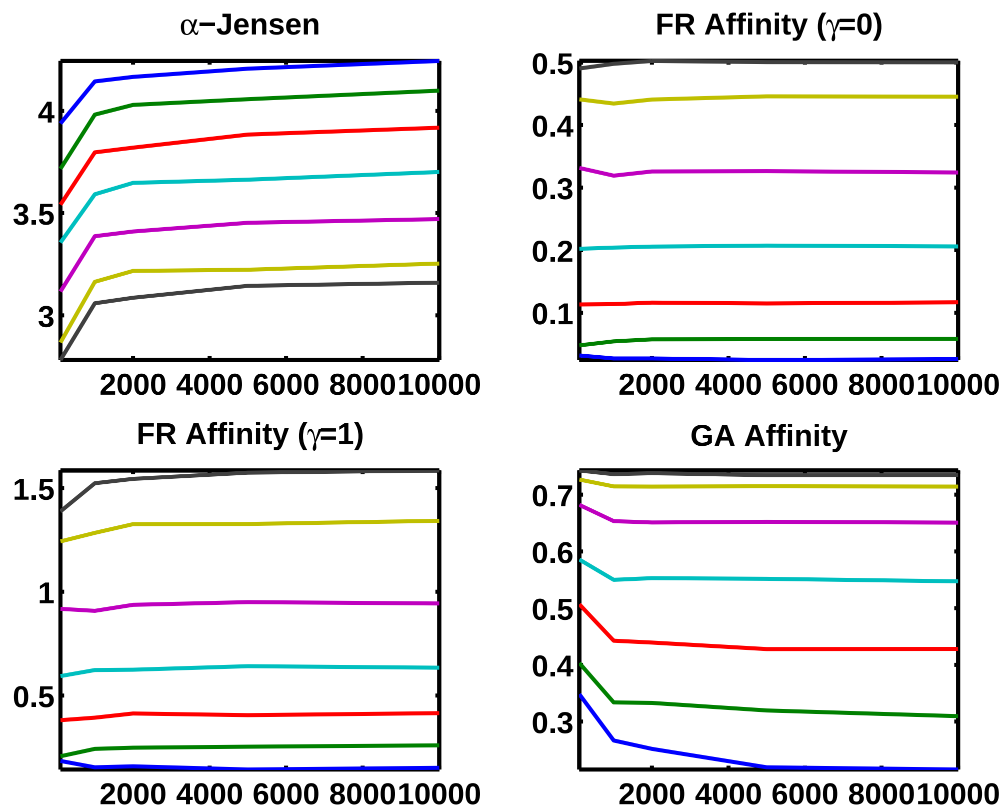
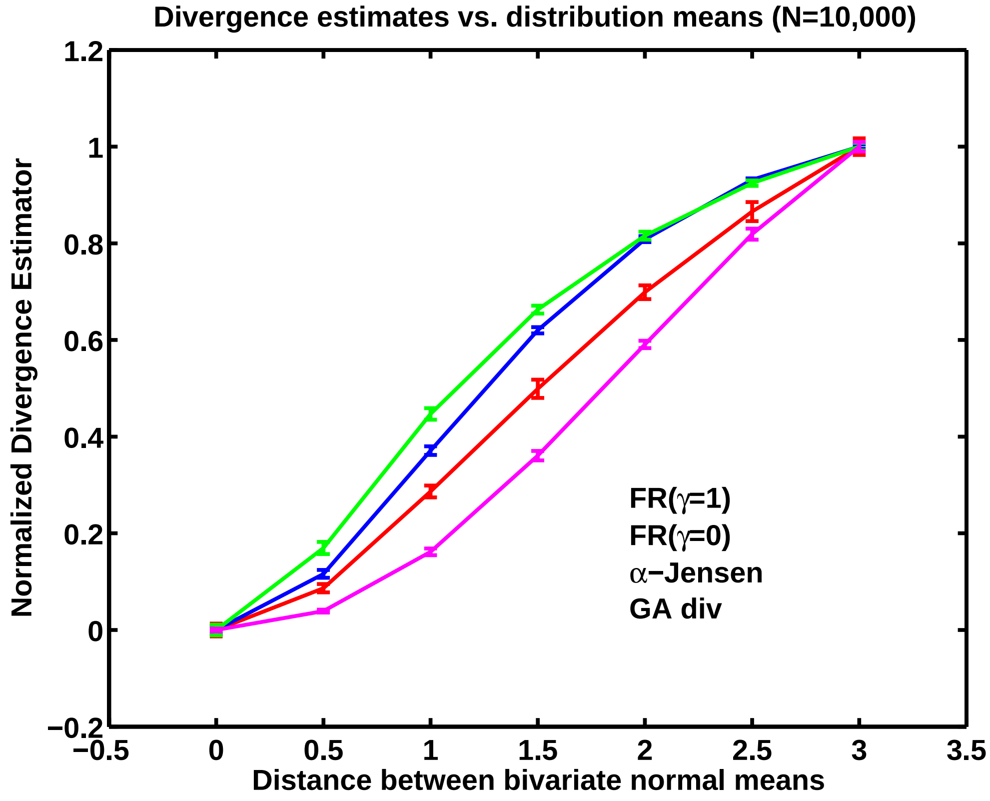
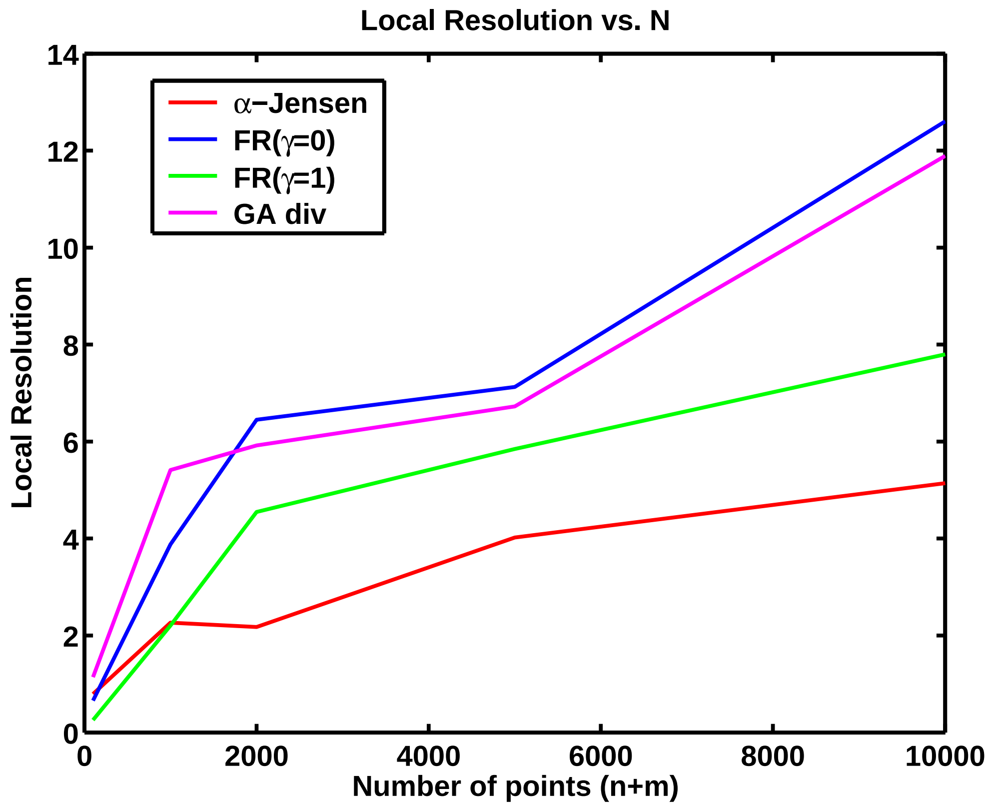


Figure 14: Convergence rates $1/\sqrt{N}$ (left) and $1/N$ (right)

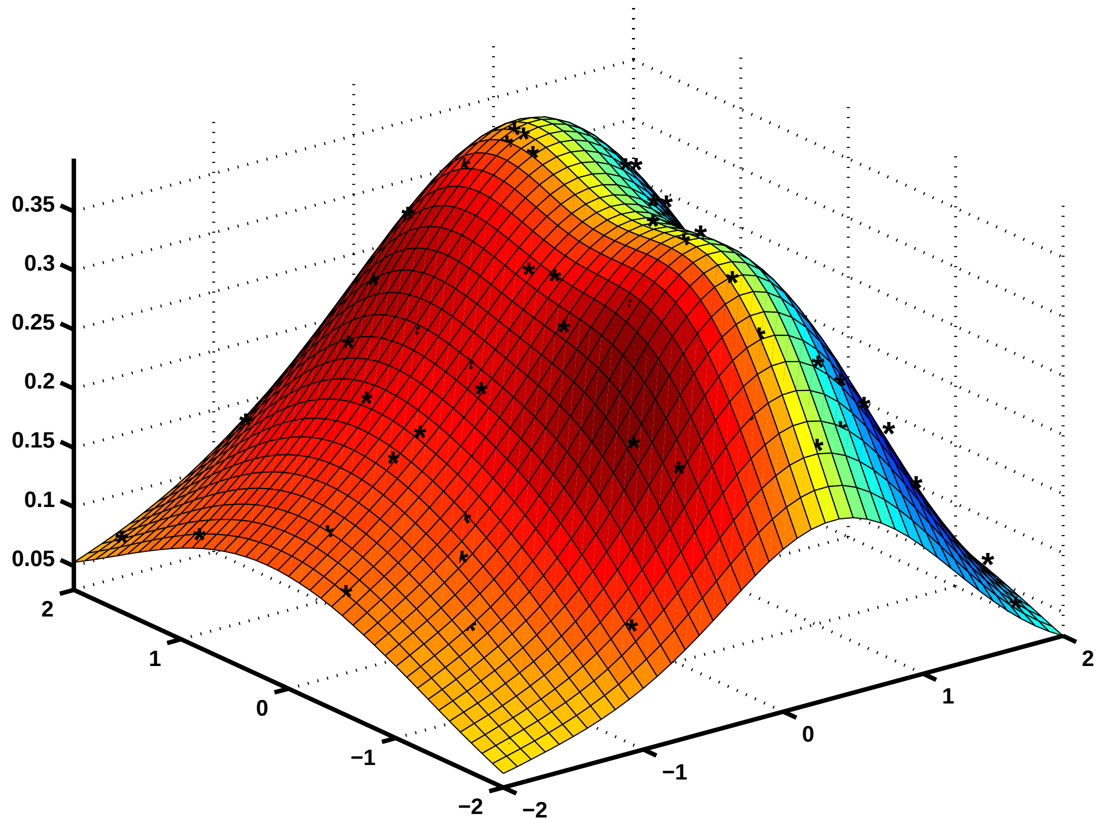
Pattern Matching Simulation: Normalized Divergence



Pattern Matching Simulation: Local Resolution



Application to Classification of Shape Manifolds



Entropy and Intrinsic Dimension on Manifolds

Focus applications: face compression and recognition, lung nodule classification, gene classification, Internet traffic characterization.

Motivation: $N \times N$ images $\{X_i\}_{i=1}^n$ of smooth shapes lie on a proper d-dimensional subspace of $\mathbf{R}^{N^2}$:

$$X_i \in S \subset \mathbf{R}^{N^2}$$

Implications:

1. *Extrinsic dimension* $N^2 >$ *Intrinsic dimension* d

2. N^2-dimensional image density $f(x)$ is concentrated on S and has *extrinsic entropy*

$$\int_{\mathbf{R}^{N^2}} f^{\alpha}(x)dx = 0$$

MST and Intrinsic Dimension

Proposition 1 *(Costa,Hero:2003) Let* $S \subset \mathbf{R}^{N^2}$ *be a* **smooth** *manifold having dimension* d_o*.Then if* $X \in \mathbf{R}^{N^2}$ *are i.i.d. realizations from a Lebesgue density* $f(x)$ *on* S*:*

$$E[L_\gamma(X_1,\ldots,X_n)]/n^{(d-\gamma)/d} \to \begin{cases} \infty, & d < d_o \\ \beta_{L_\gamma,d_o} \int_S f^{(d_o-\gamma)/d_o}(x)\mathrm{d}x, & d = d_o \\ 0, & d > d_o \end{cases}$$

$\Rightarrow$ **Estimation** of $[d, H_\alpha]$ can be accomplished via LS solution $[\hat{\alpha}, \hat{C}]$ to

$$\ln E[L_\gamma(X_1,\ldots,X_n)] = \overbrace{(d-\gamma)/d}^{\alpha} \ln n + C + \varepsilon_n, \quad n \geq n_o \ldots$$

- $\hat{d} = \gamma/(1-\hat{\alpha})$
- $\hat{H}_\alpha = \hat{C}/(1-\hat{\alpha})$

Estimation Procedure

MST resampling algorithm applied to face database:

```
Initialize:  Using entire database of face images
construct distance matrix E on face manifold via isomap
(Tenenbaum etal 2000).

For n = n_o, ..., n_1

  Repeat
     Randomly select n face images from database
     Construct MST over n face images using E matrix
  end repeat
  Compute sample average MST length \hat{L}_γ(n)

end for

Estimate d and H_α from {\hat{L}_γ(n)}_n via LS
```

Application to Yale Face Database

Figure 15: *Samples of a face from Yale database.*

- Faces of 4 persons investigated
- 585 poses and illumination conditions for each person
- extrinsic dimension = 4096, $\gamma = 1$

Application to Yale Face Database

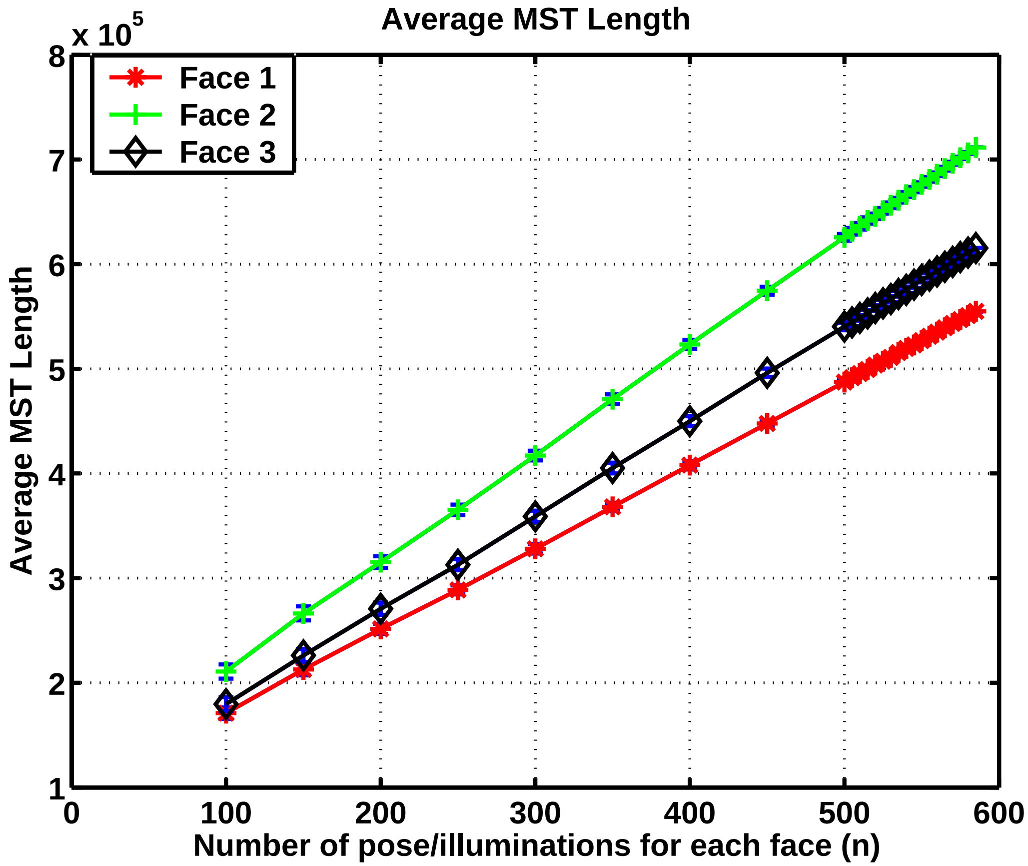


Figure 16: *Avg. intrinsic MST length for three faces.*

Application to Yale Face Database: Results

Single Faces

$\Rightarrow$ Dimension of single face manifold: $3 < \hat{d} < 4$

$\Rightarrow$ Entropy of single face manifold: $28 < \hat{H}_\alpha < 32$

Multiple Faces

$\Rightarrow$ Dimension of 3 face manifold: $\hat{d} \approx 7$

$\Rightarrow$ Entropy of 3 face manifold: $\hat{H}_\alpha \approx 60$

Conclusions

1. Entropic graphs can be used to estimate α-entropy and α-divergence
2. MST and k-NN applied to high dimensional feature-based image registration
3. Clustering using entropic K-point graphs
4. Extensions to larger class of continuous quasi-additive graphs (Yukich)
5. Can use entropic graphs to explore multivariate shape distributions
6. Can also handle case of smooth manifolds of unknown dimension

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