Semi- and Non-Parametric Mixture Models: A Progress Report

Tom Hettmansperger
Tatiana Benaglia
Tracey Wrobel
Penn State University

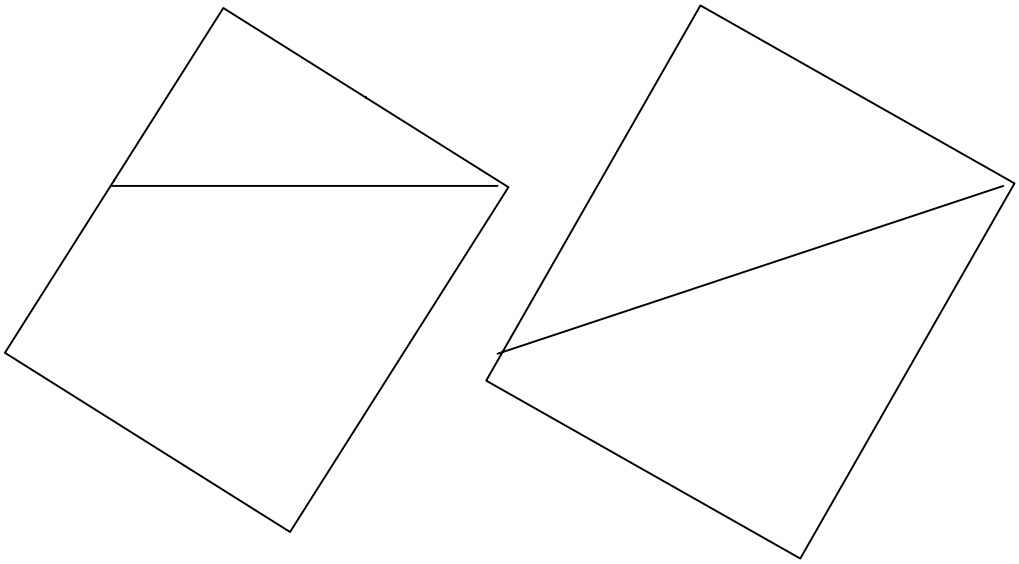
Dave Hunter
Didier Chauveau
Hoben Thomas

Current and Future Trends in Nonparametrics
October 11-12, 2007
University of South Carolina

Water Level Task

405 Children

Ages 11-16



Measurement = angular error

Clock settings: 1,2,4,5,7,8,10,11

Piaget:

Age 4: no understanding

Ages 5-7: confused but learning

Age 9: should understand

Data: 405 vectors of 8 measurements

Problem: Fit a 3 component multivariate mixture without assuming a parametric form for the underlying model

$$f(\mathbf{x}) = \lambda_1 f_1(\mathbf{x}) + \lambda_2 f_2(\mathbf{x}) + (1 - \lambda_1 - \lambda_2) f_3(\mathbf{x})$$

$\mathbf{x}$ is an 8×1 vector of measurements

We will focus on 2-component mixtures

The Model: $f(\mathbf{x}) = \lambda f_1(\mathbf{x}) + (1-\lambda) f_2(\mathbf{x})$

The Data: $\mathbf{x}_1, \ldots, \mathbf{x}_n$ $m \times 1$ vectors of measurements

The Problem: Fit the model to the data, making minimal assumptions on f_1 *and* f_2.

The Issues: Identifiability and computability

Want List: Estimates of f_1, f_2 and marginal estimates of means, standard deviations,...

Identifiability

Suppose

$$f(\mathbf{x}) = \lambda \Pi_{j=1}^{m} f_{1j}(x_j) + (1-\lambda)\Pi_{j=1}^{m} f_{2j}(x_j)$$

conditionally independent measurements but not necessairly identically distributed. No assumptions on the marginal distributions.

Result: A k-component mixture is identifiable provided $m \geq m_k$ where $m_k \geq m_k^*$ and $2^{m_k^*} - 1 \geq k m_k^* + 1.$

$$(k, m_k^*) : (2,3),\ (3,4),\ (4,5),\ (5,5)\ldots$$

Hall, Neeman, Pakyari, and Elmore (2005)

Conditional Independence

$$f(x_1, x_2) = \lambda f_{11}(x_1) f_{12}(x_2) + (1 - \lambda) f_{21}(x_1) f_{22}(x_2)$$

$$EX_1 = \lambda \mu_{11} + (1 - \lambda) \mu_{21}$$
$$EX_2 = \lambda \mu_{12} + (1 - \lambda) \mu_{22}$$

$$VarX_1 = \lambda_1 \sigma_{11}^2 + \lambda_2 \sigma_{21}^2 + \lambda_1 \lambda_2 (\mu_{11} - \mu_{21})^2$$
$$VarX_2 = \lambda_1 \sigma_{12}^2 + \lambda_2 \sigma_{22}^2 + \lambda_1 \lambda_2 (\mu_{12} - \mu_{22})^2$$

$$Cov(X_1, X_2) = \lambda_1 \lambda_2 (\mu_{11} - \mu_{21})(\mu_{12} - \mu_{22})$$

Note: $Cov(X_1, X_2) = 0$ for scale mixtures.

Let S_0 denote the estimate of the covariance matrix assuming conditional independence and let S denote the usual sample covariance matrix.

Hope: $S_0 \; and \; S$ are close.

A check on conditional independence:

Bootstrap 95% confidence interval for $\frac{\lambda_{(m)}}{\lambda^0_{(m)}}$, the ratio of maximum eigen values for S and S_0.

Want: 95% confidence interval to contain 1.

If the 95% confidence interval contains 1 then we proceed to fit the model assuming conditional independence. Otherwise, we may have identifiability problems.

A possibility: Transform $Y = S_0^{1/2} S^{-1/2} X$

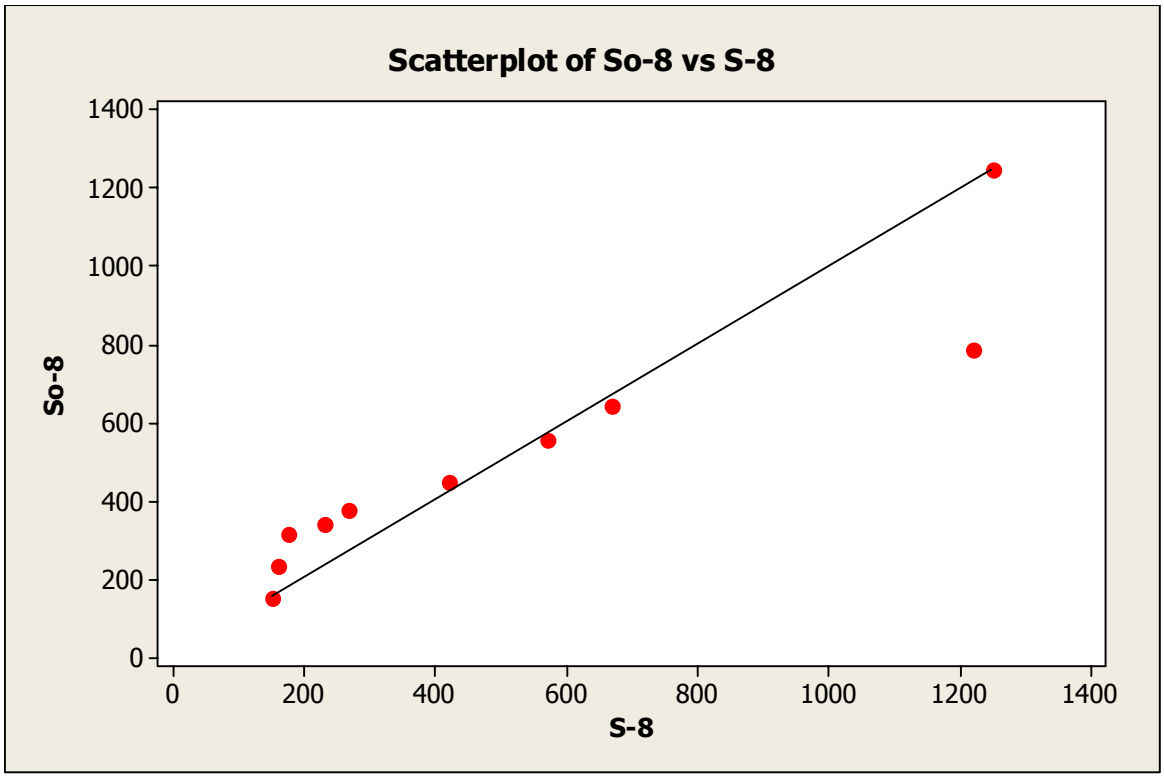
Then Y has the covariance structure roughly corresponding to conditional independence (at least conditionally uncorrelated).

Fit the conditionally independent model to the Y data. The Y data are like vectors of scores made up of linear combinations of the original measurements.

Water Level Data

Two analyses: first using all $m = 8$ measurements and secondly using $m = 4$ measurements corresponding to clock settings $1, 2, 4, 5$ on the right side of the clock.

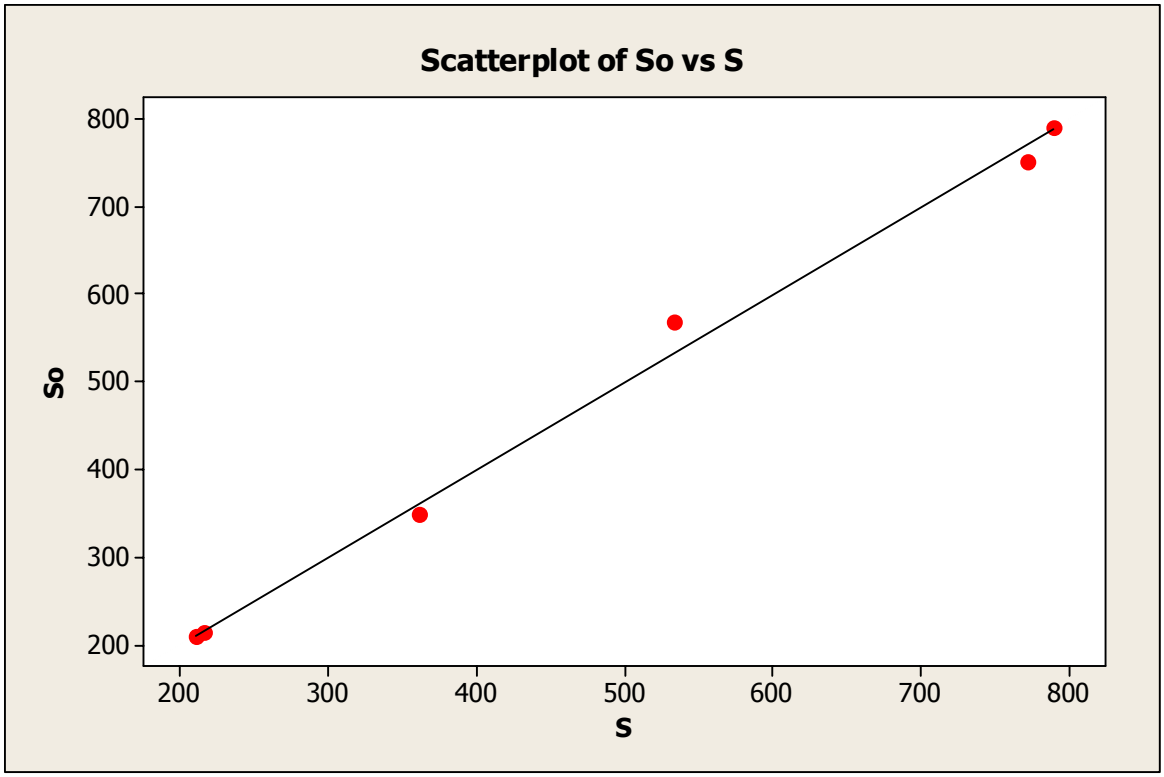
$m = 8$ measurements:



$\frac{\lambda_{(m)}}{\lambda^0_{(m)}} = 1.55$ and

95% confidence interval: $(1.15,\ 1.98)$

$m = 4$ measurements



$\frac{\lambda_{(m)}}{\lambda^0_{(m)}} = 1.03$ and

95% confidence interval: $(0.96,\ 1.28)$

$$S = \begin{pmatrix} 233 & 63 & -4 & -37 \\ 63 & 714 & -96 & -20 \\ -4 & -96 & 581 & 15 \\ -37 & -20 & 15 & 354 \end{pmatrix}$$

eigen values: $772,\ 533,\ 361,\ 216$

$$S_0 = \begin{pmatrix} 233 & 49 & -18 & -52 \\ 49 & 714 & -44 & -72 \\ -18 & -44 & 581 & 41 \\ -52 & -72 & 141 & 354 \end{pmatrix}$$

eigen values: $752,\ 569,\ 349,\ 213$

Proceed with the analysis of the 4 measurement data.

Computability

Again, the discussion will be confined to 2 components.

$$L = \prod_{i=1}^{n} (\lambda \Pi_{j=1}^{m} f_{1j}(x_{ij}) + (1-\lambda)\Pi_{j=1}^{m} f_{2j}(x_{ij}))$$

If we know which component x_{ij} belongs to then letting $z_i = 1$ if the first component and 0 otherwise, the complete likelihood is:

$$L_c = \prod_{i=1}^{n} \prod_{j=1}^{m} \{f_{1j}(x_{ij})^{z_i} f_{2j}(x_{ij})^{(1-z_i)} \lambda^{z_i} (1-\lambda)^{(1-z_i)}\}$$

"EM algorithm" next

Initial Values:

a. Use a 2-means clustering algorithm and let $z_i^{(0)} = 1$ if the vector of measurements $\mathbf{x}_i$ is in the first cluster and 0 otherwise.

Then compute $\lambda^{(0)} = ave(z_i^{(0)})$

b. Using $z_i^{(0)} \quad i = 1, \ldots n$ and $\lambda^{(0)}$ compute:

$$f_{1j}^{(0)}(u) = \frac{1}{\lambda^{(0)} nh} \sum_{i=1}^{n} z_i^{(0)} K\left(\frac{u - x_{ij}}{h} \right)$$

Similarly for $f_{2j}^{(0)}(u)$.

Updating and Iterations:

E step:

$$z_i^{(t+1)} = \frac{\lambda^{(t)} \prod_{j=1}^{m} f_{1j}^{(t)}(x_{ij})}{\lambda^{(t)} \prod_{j=1}^{m} f_{1j}^{(t)}(x_{ij}) + (1-\lambda^{(t)}) \prod_{j=1}^{m} f_{2j}^{(t)}(x_{ij})}$$

"M step"

$$\lambda^{(t+1)} = ave(z_i^{(t+1)})$$

$$\mu_{1j}^{(t+1)} = \frac{\sum_{i=1}^{n} z_i^{(t+1)} x_{ij}}{\sum_{i=1}^{n} z_i^{(t+1)}}$$

$$f_{1j}^{(t+1)}(u) = \frac{1}{\lambda^{(t+1)} nh} \sum_{i=1}^{n} z_i^{(t+1)} K\left(\frac{u - x_{ij}}{h}\right)$$

Stopping: When change in $\lambda^{(t)}$, and $\mu_{kj}^{(t)}$ $k = 1, 2$ and $j = 1, \ldots, m$ is sufficiently small.

Attractive since:

Fast to compute for general m, the number of measurements, and k, the number of components.

Performed well in simulation studies

Easy to determine features of the component marginal distributions, eg. means, medians, stdevs, pdfs, and cdfs.

Motivated by work of Bordes, Chauveau, Vandekerkhove (2007)

Water Level Data, 4 measurements

Friedman Test:

S = 237.40 DF = 3 P = 0.000

meas	n	Est med	Sum of Ranks
1	405	-0.125	1079
2	405	4.125	1297
3	405	-3.625	755.5
4	405	-1.875	918.5

Suggesting that the 4 measures are not identically distributed.

Eigen values for S_0 and S suggest that we need not reject the assumption of conditionally uncorrelated measures.

Proceed with fitting the model to the data...

4 measurements, 3 components

Means:

Meas	Comp 1	Comp 2	Comp 3
1	-1.9	0.2	21.7
2	8.5	2.0	32.0
3	-13.2	-1.8	-19.1
4	-6.2	-1.5	-31.9

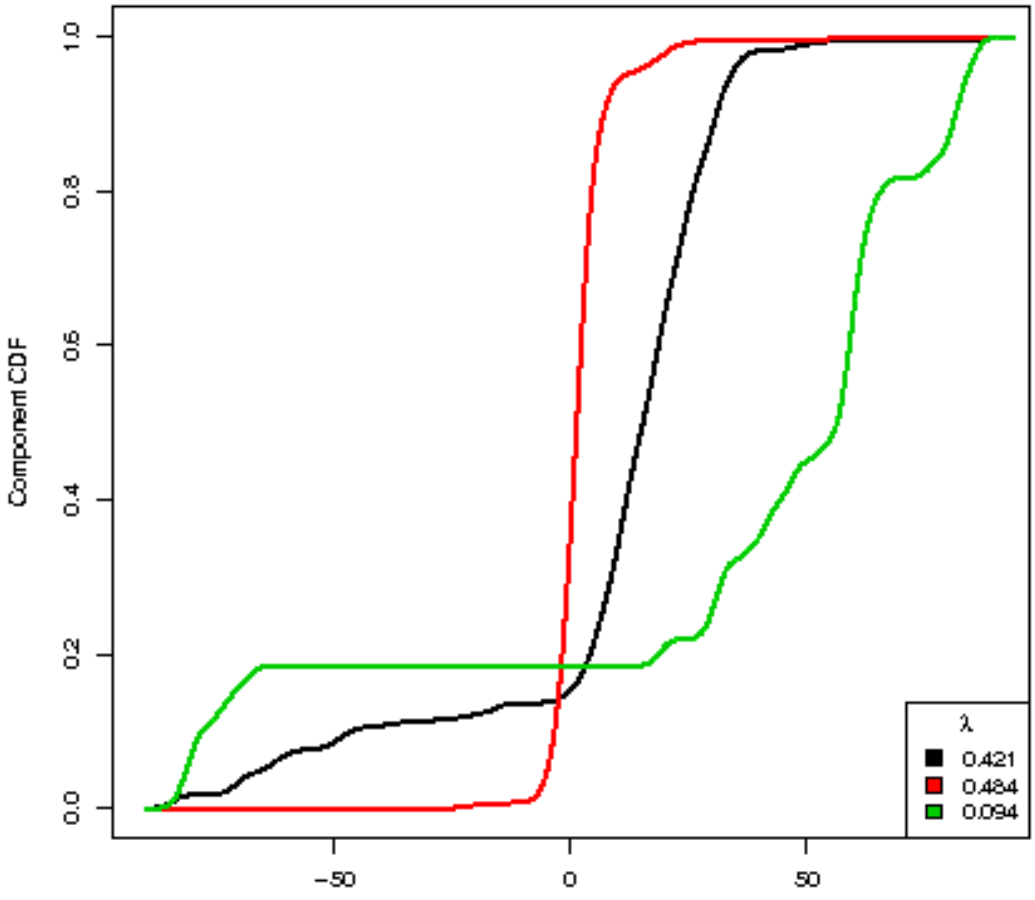
Standard Deviations:

Meas	Comp 1	Comp 2	Comp 3
1	15.9	6.4	25.8
2	28.5	6.4	54.5
3	23.0	6.5	56.0
4	23.4	6.9	17.3

Lambdas: .42, .49, .09

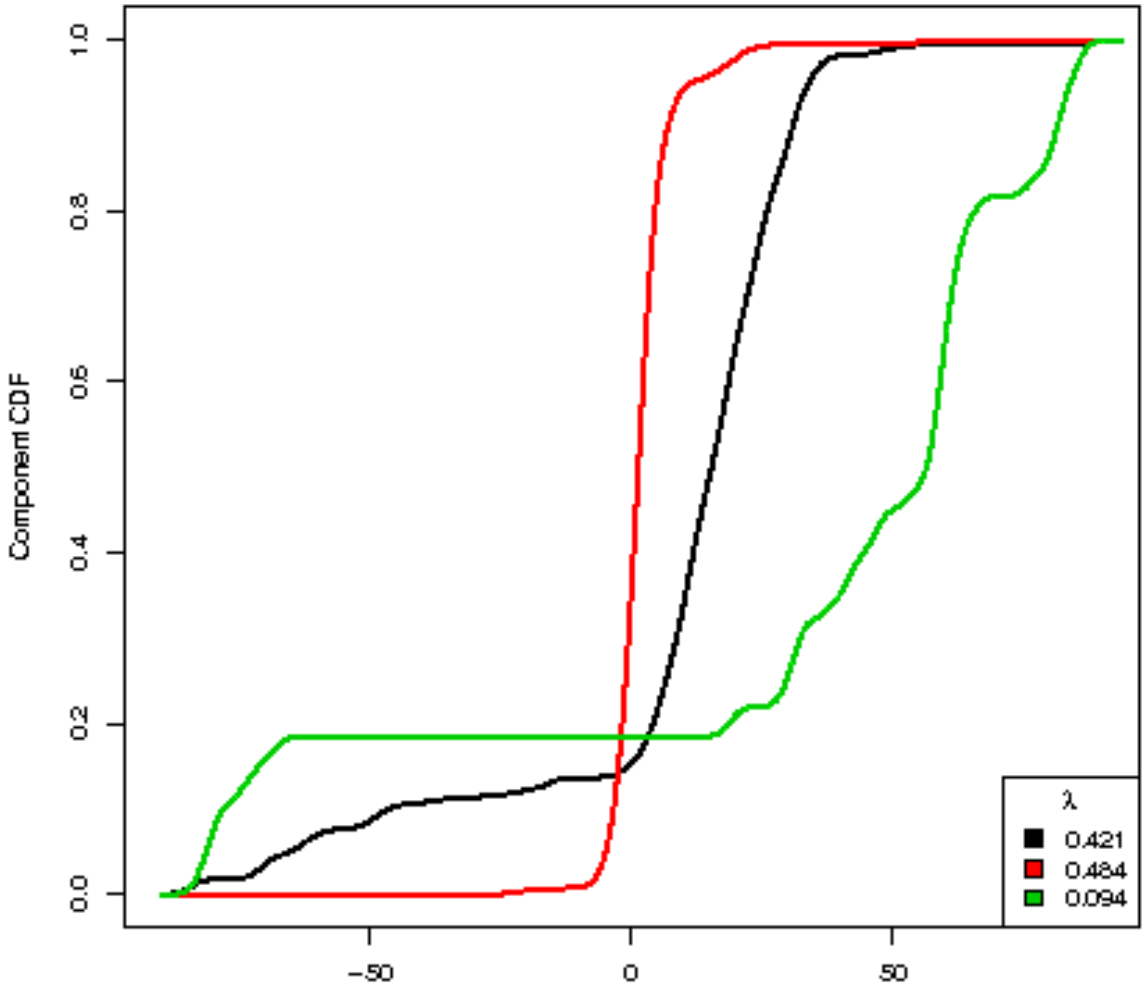
CDF plots for the first measurement

1 o’clock



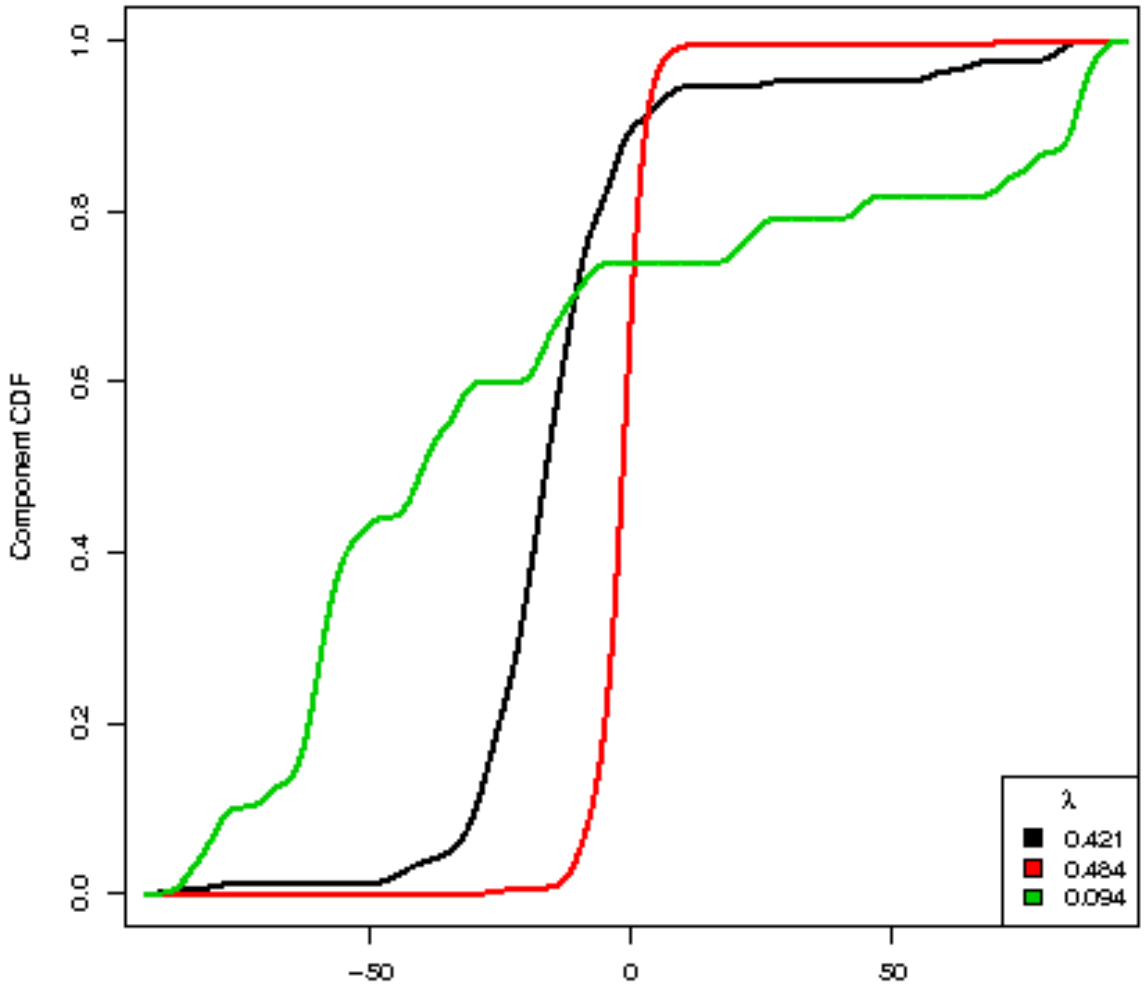
CDF plots for the second measurement

2 o’clock



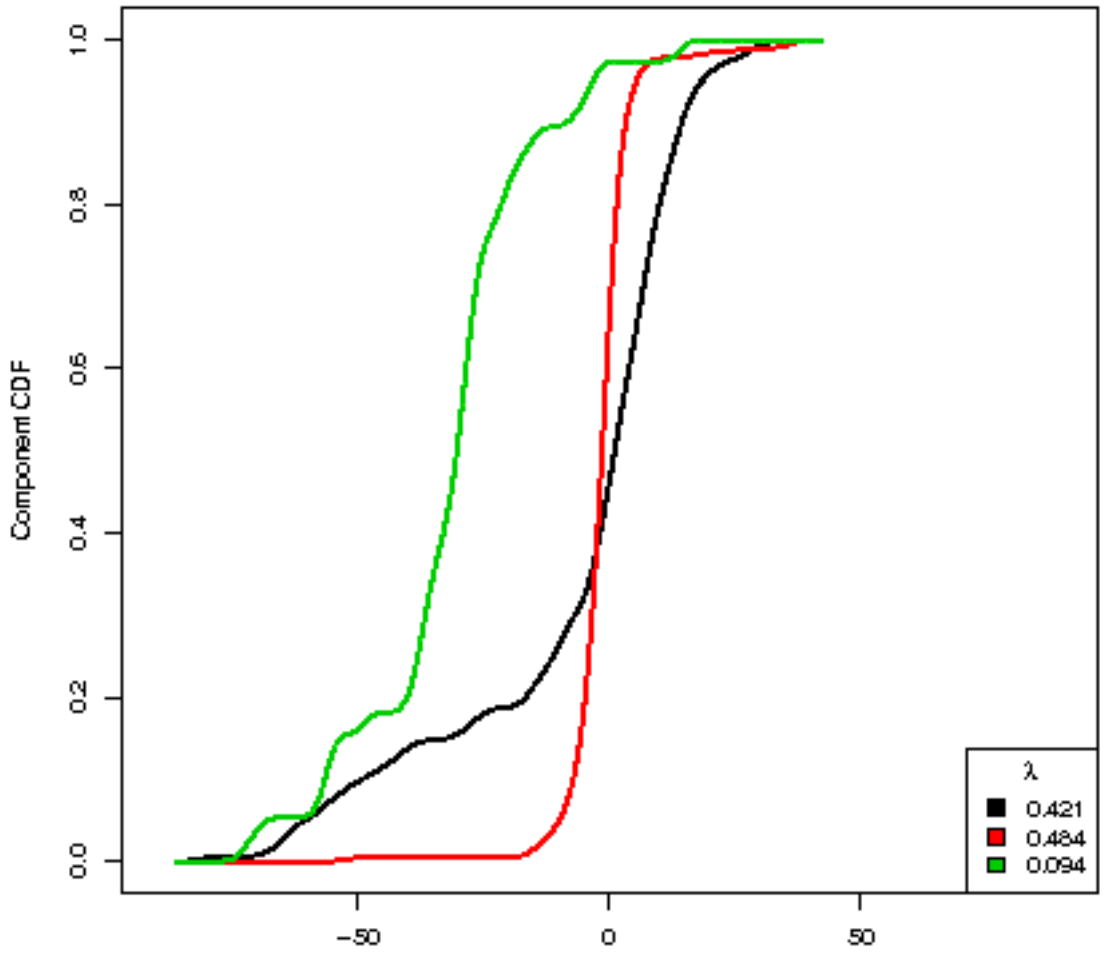
CDF plots for the third measurement

4 o’clock

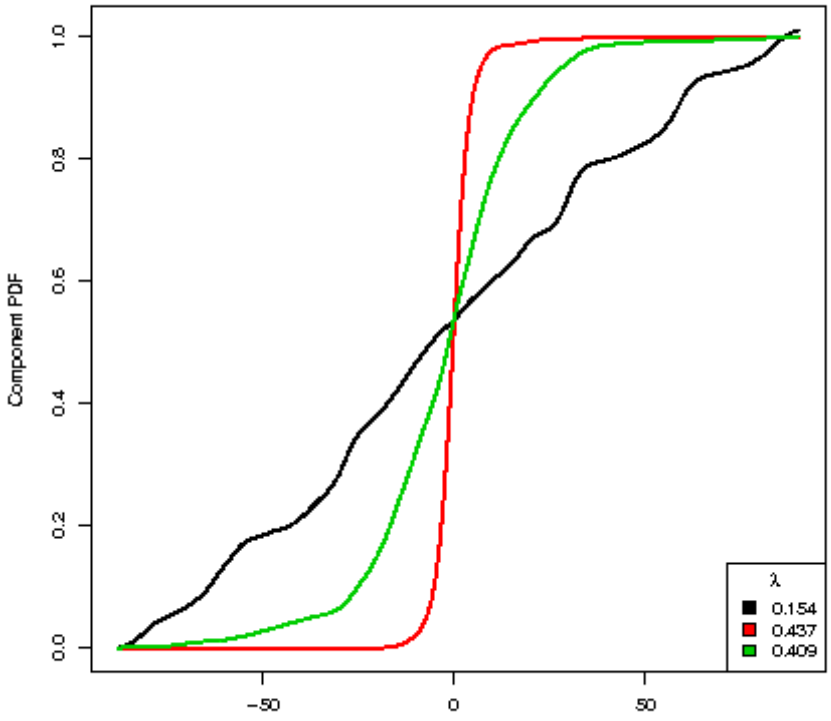


CDF plots for the fourth measurement

5 o’clock



If we assume iid measures, then the 4 plots are combined:



Mean	-1.8	-.1	-2.6
Stdev	45.8	4.9	20.7
Lambda	.15	.44	.41

Other work: Qin and Leung (2006)

2 components and 3 measurements

Conditionally independent model:

$$f(\mathbf{x}) = \lambda \Pi_{j=1}^{3} f_j(x_j) + (1-\lambda)\Pi_{j=1}^{3} g_j(x_j)$$

Exponential tilt:

$$g(x_j) = f_j(x_j)\exp(\beta_{0j} + \beta_{1j}x_j + \beta_{2j}x_j^2)$$

The algorithm:

1. determine initial values for $\lambda,\ \beta_{0j}, \beta_{1j}, \beta_{2j}$ $j = 1,2,3$

2. use empirical likelihood to estimate F_j

3. use EM to estimate $\lambda,\ \beta_{0j}, \beta_{1j}, \beta_{2j}$ $j = 1,2,3$

$$L = \prod_{i=1}^{n}\prod_{j=1}^{3}\left(\lambda + (1-\lambda)e^{\beta_{0j}+\beta_{1j}x_j+\beta_{2j}x_j^2}\right)dF_j(x_{ij})$$

The Univariate Case

Identifiability:

Model:

$$f(x) = \lambda g(x - \mu_1) + (1 - \lambda) g(x - \mu_2)$$

where g is symmetric about 0.

Hunter, Wang, Hett. (2007)

Bordes, Mottelet, Vandekerkhove (2006)

Computatability:

Very expensive. Algorithms only for 2 component case.

Two possiblities:

1. "EM" algorithm (Bordes, Chauveau,Vandekerkhove (2007))

Suppose we have initial values for μ_1, μ_2, and $g(.)$.

E step

$$z_i^{(t+1)} = \frac{\lambda^{(t)} g^{(t)}(x_i - \mu_1^{(t)})}{\lambda^{(t)} g^{(t)}(x_i - \mu_1^{(t)}) + (1 - \lambda^{(t)}) g^{(t)}(x_i - \mu_2^{(t)})}$$

"M step"

$$\lambda^{(t+1)} = ave(z_i^{(t+1)}) \; and \; \mu_1^{(t+1)} = ave(z_i^{(t+1)} x_i)$$

$$g^{(t+1)}(u) = \frac{1}{2nh} \sum_{i=1}^{n} \sum_{j=1}^{2} z_{ij}^{(t+1)} \{K\left(\frac{u - x_i - \mu_j^{(t+1)}}{h} \right)$$

$$+ K\left(\frac{-u - x_i - \mu_j^{(t+1)}}{h} \right)\}$$

2. Exponential Tilt Model

$$f(x) = \lambda g_0(x) e^{\beta_{01}+\beta_{11}x+\beta_{21}x^2} +$$

$$(1-\lambda) g_0(x) e^{\beta_{02}+\beta_{12}x+\beta_{22}x^2}$$

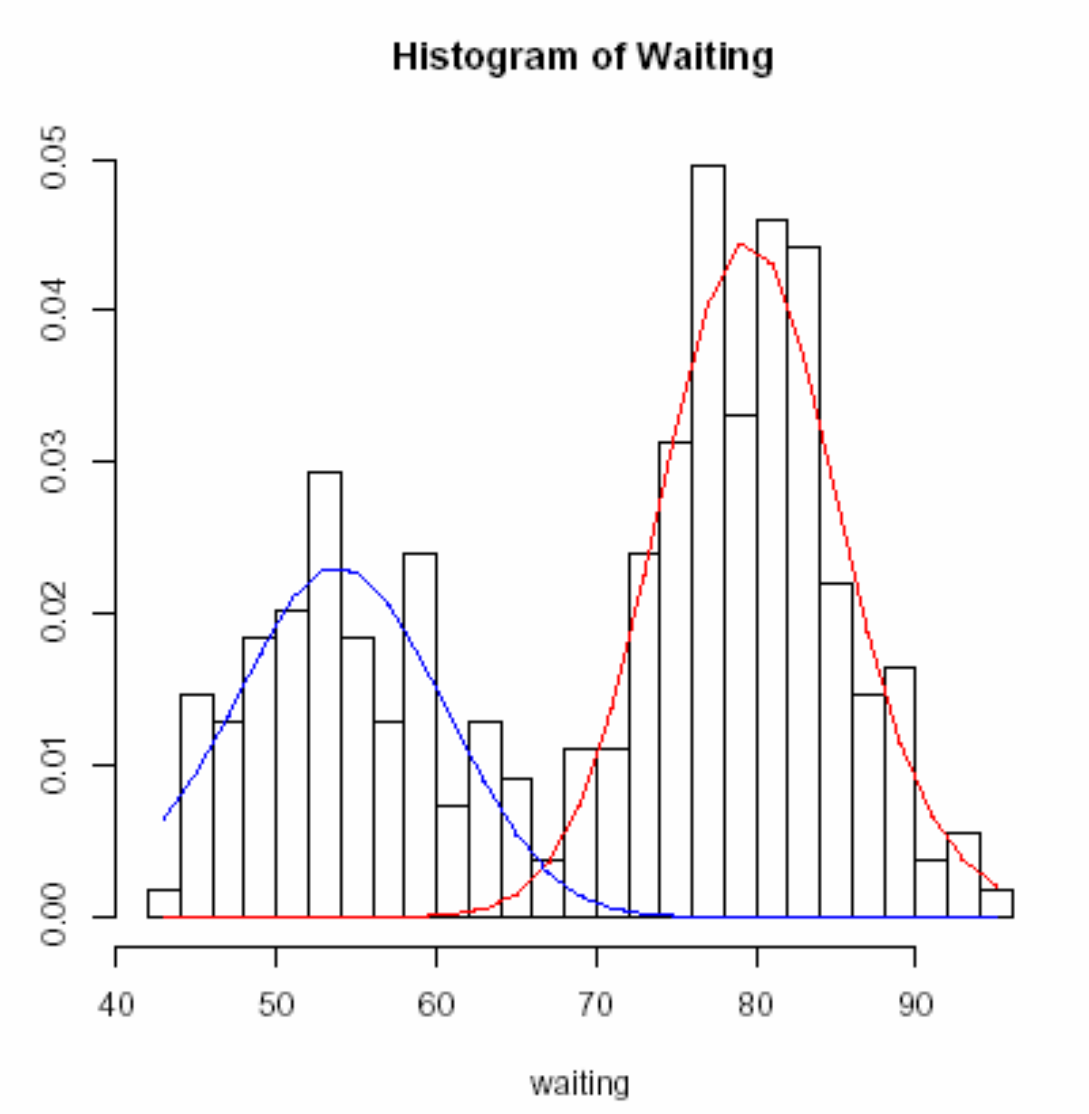
$g_0(x)$ is called the carrier density.

Motivated by Efron and Tibshirani (1996) in the non-mixture case.

Computation: discretize the data, use a kernel density estimator for $g_0(x)$, and an EM algorithm to estimate βs. Computation is carried out via a mixture of Poisson regressions.

Computation is fast and works for k components.

Example: Time between eruptions of Old Faithful Geyser



Issues: identifiability, estimation of the carrier...

The End