

Feature network models for proximity data: statistical inference, model selection, network representations and links with related models

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Feature Network Models for Proximity Data

Statistical inference, model selection, network representations and links with related models

PROEFSCHRIFT

ter verkrijging van de graad van Doctor aan de Universiteit Leiden, op gezag van de Rector Magnificus Dr. D.D. Breimer, hoogleraar in de faculteit der Wiskunde en Natuurwetenschappen en die der Geneeskunde, volgens besluit van het College voor Promoties te verdedigen op donderdag 21 september 2006 klokke 13.45 uur

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Laurence Emmanuelle Frank

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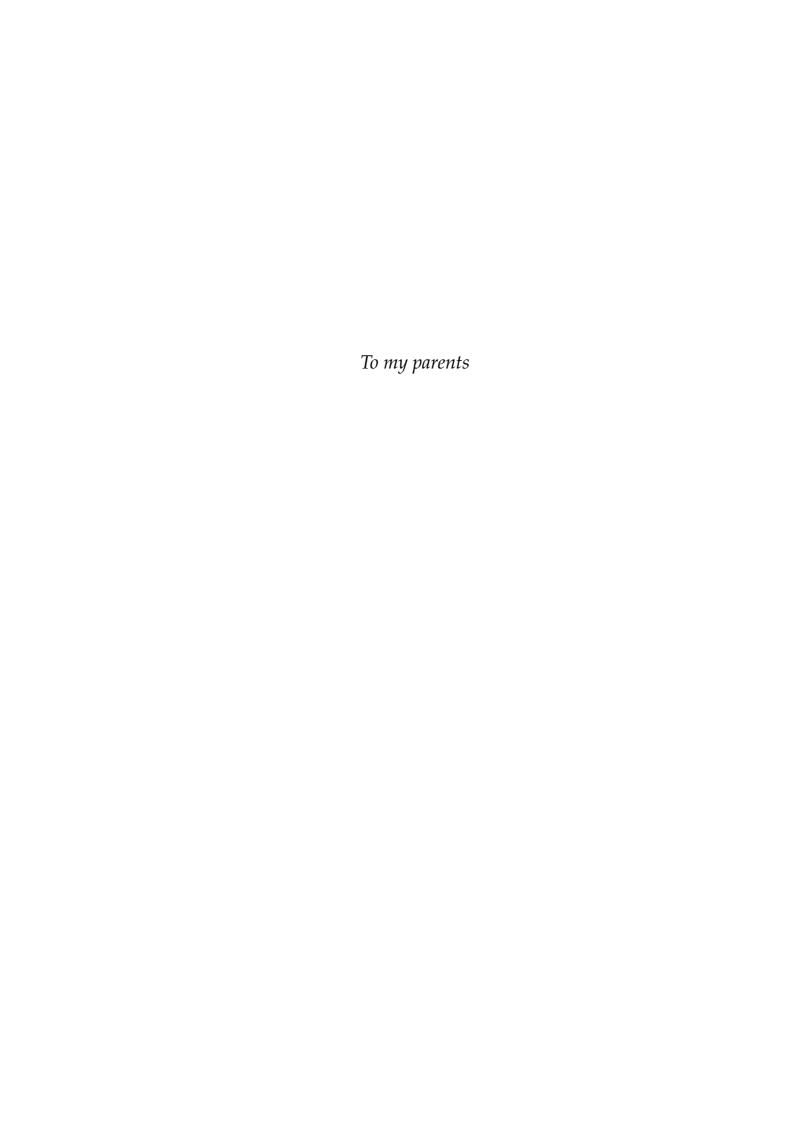
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"On ne peut se flatter d'avoir le dernier mot d'une théorie, tant qu'on ne peut pas l'expliquer en peu de paroles à un passant dans la rue."

[It is not possible to feel satisfied at having said the last word about some theory as long as it cannot be explained in a few words to any passer-by encountered in the street.]

Joseph Diaz Gergonne, French mathematician (Chasles, 1875, p. 115).

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Notation and Symbols

Notation conventions

matrices: bold capital vectors: bold lowercase scalars, integers: lowercase

Symbols

Symbol	Description
0	an object or stimulus
m	the number of objects, stimuli
i	$index i = 1, \cdots, m$
i	$index j = 1, \cdots, m$
k	$index k = 1, \cdots, m$
n	the number of object pairs = $\frac{1}{2}m(m-1)$
1	$index l = 1, \cdots, n$
N	the number of replications of samples of size $n \times 1$
ℓ	$index \ell = 1, \cdots, N$
f	a frequency value associated with an object pair
$egin{array}{c} f \ \delta \ \hat{\delta} \end{array}$	a dissimilarity value associated with an object pair
	an estimated dissimilarity value associated with an object pair
δ	an $n \times 1$ vector with dissimilarities between all object pairs
$oldsymbol{\delta}$ $oldsymbol{\hat{\delta}}$ $oldsymbol{\Delta}$ $oldsymbol{\widetilde{\Delta}}_{l\ell}$ $oldsymbol{\widetilde{\Delta}}_{l}$	an $n \times 1$ vector with estimated dissimilarities between all object pairs
<u>Δ</u>	an $m \times m$ matrix with dissimilarities
$\Delta_{l\ell}$	a random variable producing realisations $ ilde{\delta}_{l\ell}$
$ ilde{\delta}_{l\ell}$	a realisation of random variable $\widetilde{\Delta}_{l\ell}$
$\widetilde{oldsymbol{\Delta}}$	an $n \times N$ matrix of random variables $\widetilde{\Delta}_{l\ell}$
$\overline{\Delta}_{l}$	mean of a row l of $\widetilde{\Delta}$
	a similarity value associated with an object pair
ç	an $n \times 1$ vector with similarities between all object pairs
$arsigma _{oldsymbol{arsigma} _{oldsymbol{arsigma} }}^{oldsymbol{arsigma} }$ $oldsymbol{arsigma} _{oldsymbol{arsigma} }$	an $m \times m$ matrix with similarities
	a feature, which is a binary $(0,1)$ vector of size $m \times 1$
$F_{\rm C}$	a <i>cluster</i> feature, which is a binary $(0,1)$ vector of size $m \times 1$
$F_{ m U}$	a <i>unique</i> feature, which is a binary $(0,1)$ vector of size $m \times 1$
T	the number of features

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T_{\rm C}
                   the number of cluster features
T_{\rm U}
                   the number of unique features
                   the total number of distinctive features = \frac{1}{2}(2^m) - 1
T_{\mathcal{D}}
                   index for the features: t = 1, \dots, T
t.
                   index for the cluster features: t_C = 1, \dots, T_C
t_{\rm C}
                   index for the unique features: t_U = 1, \dots, T_U
t_{\rm II}
S_i
                   the set of features that represents object O_i
E
                   an m \times T matrix with columns representing features
                   a row vector from the matrix E
e
                   an element of the matrix E
е
\mathbf{E}_T
                   an E matrix with special feature structure that yields a tree representation
                   the part of \mathbf{E}_T (size m \times T_{\rm C}) that represents the set of cluster features
\mathbf{E}_{C}
                   the part of \mathbf{E}_T (size m \times T_U) that represents the set of unique features
\mathbf{E}_{U}
X
                   an n \times T matrix with featurewise distances obtained with \mathbf{x}' = |\mathbf{e}_{it} - \mathbf{e}_{it}|
\mathbf{x}'
                   a row vector from the matrix X
                   a column vector from the matrix X
X
                   an n \times T_C + T_U matrix with featurewise distances obtained with \mathbf{E}_T
\mathbf{X}_T
\mathcal{D}
                   the complete set of featurewise distances
d
                   a distance between an object pair
d
                   an n \times 1 vector of distances between all object pairs
â
                   an n \times 1 vector of estimated distances between all object pairs
đτ
                   an n \times 1 vector of estimated distances between all object
                   pairs for a tree structure
                   feature discriminability parameter
η
                   true value of ordinary least squares feature discriminability parameter
\eta_{\mathrm{OLS}}
                   true value of inequality constrained least squares
\eta_{\rm ICLS}
                   feature discriminability parameter
                   true value of Lasso feature discriminability parameter
\eta_{\rm L}
\eta_{\mathrm{PL}}
                   true value of Positive Lasso feature discriminability parameter
                   an T \times 1 vector of feature discriminability parameters
                   an T \times 1 vector of true values \eta_{OLS}
\eta_{
m OLS}
                   an T \times 1 vector of true values \eta_{ICLS}
\eta_{\text{ICLS}}
                   an T \times 1 vector of true values \eta_L
\eta_{\rm L}
                   an T \times 1 vector of true values \eta_{PL}
\eta_{\rm PL}
                   estimated values of \eta, \eta_{\text{OLS}}, \eta_{\text{ICLS}}, \eta_{\text{L}}, \eta_{\text{PL}}
\hat{\eta}, \hat{\eta}_{OLS}
                   the number of constraints necessary to obtain \hat{\pmb{\eta}}_{\text{ICLS}}
C
С
                   index c = 1, \dots, C
r
                   a C \times 1 vector with constraints
Α
                   a C \times T matrix of constraints of rank c
                   a m \times 1 vector with Kuhn-Tucker mutipliers
\lambda_{\rm KT}
                   a n \times 1 vector with error values (\boldsymbol{\epsilon} = \boldsymbol{\delta} - \boldsymbol{X}\boldsymbol{\eta})
\hat{oldsymbol{\epsilon}}
                   a n \times 1 vector with estimated error values (\hat{\boldsymbol{\epsilon}} = \boldsymbol{\delta} - \mathbf{X}\hat{\boldsymbol{\eta}})
                   an element from the vector \hat{m{\epsilon}}
                   true variance and standard deviation of \epsilon
                   estimated variance and standard deviation of \hat{m{\epsilon}}
                   true variance and standard error of \eta
\hat{\sigma}_{\eta}^{2}, \hat{\sigma}_{\eta}

\hat{\sigma}_{\hat{\eta}}^{2}, \hat{\sigma}_{\hat{\eta}}

\sigma_{\text{OLS}}^{2}, \sigma_{\text{OLS}}
                   estimated nominal variance and estimated nominal standard error of \eta
                   estimated nominal variance and nominal standard error of \hat{\eta}
                   true variance and standard error of \hat{\eta}_{OLS}
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Symbols xxiii

â ² â	estimated variance and standard error of the
$\nu_{\rm QLS}, \nu_{\rm OLS}$	estimated variance and standard error of $\hat{\eta}_{ ext{OLS}}$
$\hat{\sigma}_{ ext{OLS}}^2, \hat{\sigma}_{ ext{OLS}} \ \sigma_{ ext{ICLS}}^2, \sigma_{ ext{ICLS}}$	true variance and standard error of $\hat{\eta}_{ ext{ICLS}}$
$\hat{\sigma}_{\text{ICLS}}^2, \hat{\sigma}_{\text{ICLS}}$	estimated variance and standard error of $\hat{\eta}_{\text{ICLS}}$
B	number of bootstrap samples
b	$index b = 1, \cdots, B$
\mathbf{b}_b	a bootstrap sample ($n \times 1$ vector)
$egin{array}{c} \mathbf{b}_b^* \ ilde{\mathbf{b}}_b \end{array}$	a bootstrap sample, multivariate
$ ilde{\mathbf{b}}_b$	a bootstrap sample, with sampled residuals
sd_B	standard deviation of <i>B</i> bootstrap samples
S	number of simulation samples
а	index $a = 1, \dots, S$
\mathbf{s}^*	a simulation sample ($n \times 1$ vector)
к, р	parameters binomial distribution
ĠĊV	generalized cross-validation statistic
	e .
$GCV_{ ext{FNM}}$	GCV using inequality constrained least squares estimation