

Composite likelihood for space-time data¹

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Bruce Lindsay



March 7, 1947 - May 5, 2015

Lindsay, B.G. (1988). Composite Likelihood Methods. *Contemporary Mathematics* **80**, 221-239



General framework

- In several cases models have complex interdependencies and/or we deal with large dataset.
- Joint distribution of the data may be difficult to evaluate, or even to specify!
- Typical difficulties arise from the need to invert large matrices when we deal with large dataset and/or from approximation of intractable integrals
- Ancient Roman's principle:

dividi et impera

('diviser pour regner', Louis XI)

- Idea: if computing likelihoods for certain subsets of the data is possible, then one may construct a pseudolikelihood by combining such likelihood objects and use this as a surrogate for the ordinary likelihood
- Review paper: Varin et al. (2011)



Example: spatio-temporal Gaussian data I

- $s \in \mathbb{R}^d$ is a spatial location, $t \in \mathbb{R}$ is a time point
- Observations $\mathbf{z} = (z(s_1, t_1), \dots, z(s_n, t_n))'$ from a Gaussian Random Field (GRF) $\{Z(s, t)\}$
- Weakly stationarity

$$\operatorname{cov}(Z(s,t),Z(s',t'))=C(h,u;\theta)$$

$$(h = s - s', \text{ spatial lag, } u = t - t' \text{ temporal lag}).$$

- Likelihood computation requires inversion of $n \times n$ covariance
 - $O(n^3)$ operations, $O(n^2)$ memory
 - If n large, this may be unfeasible!



Example: spatio-temporal Gaussian data II

- Two possible strategies:
 - 1. simplify the model:
 - approximate with a Gaussian Markov Random Field (Lindgren et al., 2011) requiring roughly O(n log n) operations
 - approximate with low rank methods (Cressie and Johannesson, 2008) O(n)
 - 2. keep your model but simplify the fitting method: e.g. Curriero and Lele (1999) estimate θ from the pseudolikelihood

$$PL(\theta; \mathbf{z}) = \prod_{i>j} f(z(s_i, t_i) - z(s_j, t_j); \theta) w(s_i, t_j, s_j, t_j)$$



Example: spatio-temporal non-gaussian data l

• Generalized linear geostatistical models (latent Gaussian models)

$$E(Z(s,t)|U(s,t)) = g^{-1}\left(x(s,t)'\beta + U(s,t)\right)$$

where $\{U(s, t)\}$ is a latent GRF.

• In general, the likelihood involves an n-dimensional integral

$$L(\beta,\psi,\theta;\mathbf{z}) = \int_{\mathbb{R}^n} f(\mathbf{z}|\mathbf{u};\beta,\psi) f(\mathbf{u};\theta) d\mathbf{u}$$

- Monte Carlo methods: MCEM, MCMC, etc. may be time-consuming even for moderate *n*
 - ▶ INLA method (Rue et al., 2009) ⇒ see Thomas's talk
- Simpler: pseudolikelihood constructed from bivariate margins

$$PL(\theta; \mathbf{z}) = \prod_{i>j} f(z(s_i, t_i), z(s_j, t_j); \theta)^{w(s_i, t_j, s_j, t_j)}$$



Example: spatio-temporal extreme values I

- Observations z = (z(s₁, t₁),..., z(s_n, t_n))' are maxima recorded values
- Classical extreme value theory says that the marginal distribution can be modeled by the GEV distribution

$$\Pr(Z(s,t) \leq z) = \exp\left[-\{1+\xi(z-\mu)/\sigma\}^{-1/\xi}
ight]$$

with $\mu \in \mathbb{R}$, $\xi \in \mathbb{R}$, $\sigma > 0$ and $\{1 + \xi(z - \mu)/\sigma\} > 0$.

• Unit Fréchet margins (i.e. $\mu = \xi = \sigma = 1$)

$$\Pr(Z(s,t) \leq z) = \exp[-1/z]$$



Example: spatio-temporal extreme values II

- A max-stable process (de Haan, 1984), is the extension for maxima of independent replications of (space-time) random fields.
- Suppose unit Fréchet margins. Finite dimesional distribution

$$\begin{aligned} \mathsf{Pr}(\mathbf{Z} \leq \mathbf{z}) &= \mathsf{Pr}(Z(s_1, t_1) \leq z_1, \dots, Z(s_n, t_n) \leq z_n) \\ &= \exp(-V(\mathbf{z})) \end{aligned}$$

V(z) is a positive function such that $V(a^{-1}z) = aV(z)$ for any a > 0 and z > 0

• Assume a parametric model

$$\Pr(\mathbf{Z} \leq \mathbf{z}) = \exp(-V(\mathbf{z}; \theta))$$

the likelihood corresponds to the derivative with respect to all components of $\boldsymbol{z}.$

► The number of terms is the B_n Bell number, around 8.3 × 10¹⁰ for n = 17 !



Composite likelihood: definition

Consider

- 1. a statistical model $\{f(\mathbf{z}; \theta), \mathbf{z} \in \mathbb{R}^n, \theta \in \Theta \subseteq \mathbb{R}^p\};$
- 2. a set of measurable events $\{A_k; k = 1, \dots, K\};$
- 3. the associated likelihoods $\mathcal{L}_k(\theta; \mathbf{z}) = f(\mathbf{z} \in \mathcal{A}_k; \theta)$.

Then, a composite likelihood (CL) is the weighted product of the likelihoods corresponding to each single event,

$$\mathsf{CL}(\theta; \mathbf{z}) = \prod_{k=1}^{K} \mathcal{L}_k(\theta; \mathbf{z})^{w_k},$$

where $\{w_k; k = 1, \ldots, K\}$ are positive weights.



Composite conditional likelihood

• Notation $z_i = z(s_i, t_i)$, $\mathbf{z}_D = \{z_j, j \in D\}$, $D \subset \{1, \ldots, n\}$ and \mathcal{D} is a set of D.

$$CCL(\theta; \mathbf{z}) = \prod_{D \in \mathcal{D}} f(\mathbf{z}_D | \mathbf{z}_{D^c}; \theta),$$

• Besag's pseudolikelihood (Besag, 1974)

$$CCL(\theta; \mathbf{z}) = \prod_{i=1}^{n} f(z(s_i)|\mathbf{z}_{\partial i}; \theta),$$

 ∂_i neighborhood of s_i

- Spatial GRF: Vecchia (1988), Stein et al. (2004)
- Limited number of space-time applications
 - Mixed states spatio-temporal auto-models on regular lattice (Hardouin and Crivelli, 2011)



Composite marginal likelihood

• More commonly used

$$CML(\theta; \mathbf{z}) = \prod_{D \in \mathcal{D}} f(\mathbf{z}_D; \theta)$$

- Independence likelihood (Smith, 1990; Chandler and Bate, 2007) where the sets *D* are disjoint
 - $\theta = (\theta_S, \theta_T)'$ and inference about θ_S

$$CML(\theta; \mathbf{z}) = \prod_{t=1}^{l} f(\mathbf{z}(t); \theta_{S})$$

with $z(t) = (z(s_1, t), ..., z(s_k, t))$

- pairwise likelihood: $\prod_{i>i} f(z_i, z_j; \theta)$
- tripletwise likelihood, ..., "blockwise" likelihood
- pairwise differences (for GRF): $\prod f(z_i z_j; \theta)$



Hybrid methods

- hybrid pairwise likelihood: Kuk (2007)
 - optimal estimating equations for marginal parameters
 - pairwise likelihoods for estimating dependence parameters
 - no examples for space-time examples yet !
- joint composite estimating functions : Bai et al. (2012)
 - space-time example, see later.



Composite likelihood quantities I

• Composite log-likelihood

$$c\ell(\theta; \mathbf{z}) = \log CL(\theta; \mathbf{z}) = \sum_{k}^{M} \log \ell_{k}(\theta; \mathbf{z}) w_{k}$$

• Composite score

$$u(\theta; \mathbf{z}) = \sum_{k=1}^{K} \log \nabla \ell_k(\theta; \mathbf{z}) w_k = \sum_{k=1}^{K} u_k(\theta; \mathbf{z}) w_k, \Rightarrow E[u(\theta; \mathbf{Z})] = 0$$

• Maximum composite estimator $\hat{\theta}_{CL}$

$$c\ell(\hat{ heta}_{\mathit{CL}}; \mathbf{z}) \geq c\ell(heta; \mathbf{z}), \qquad orall heta \in \Theta$$



Composite likelihood quantities II

• Godambe (or sandwich) information

 $G(\theta) = H(\theta)J(\theta)^{-1}H(\theta)$



• Sensitivity matrix: $H(\theta) = E[-\nabla u(\theta; \mathbf{Z})],$

$$\hat{H} = -\nabla u(\hat{ heta}_{CL}; \mathbf{z})$$

- Variability matrix: J(θ) = Var[u(θ; Z)] How to estimate ?
- Misspecification $H(\theta) \neq J(\theta)$



Asymptotics I

- Two types of asymptotic frameworks
 - fixed domain

b

- fill a space-time region with a sequence of observed locations
- no results
- increasing domain:
 - expand a a space-time region for recover more observed locations

• regular lattice:
$$R_0 \subset (-\frac{1}{2}, \frac{1}{2}]^{d+1}$$
,
 $R_n = \{(s_1, t_1), \dots, (s_n, t_n)\} = (\lambda_n R_0) \cap \mathbb{Z}^{d+1}$



Asymptotics II

• Idea: log-composite likelihood is an additive contrast function (Hardouin, 1992; Guyon, 1995)

$$U_n(heta) = rac{1}{K_n} \sum_{k=1}^{K_n} \log f(\mathbf{z} \in A_k; heta) w_k$$

- mixing conditions on $\{Z(s,t)\}$
- $\hat{\theta}_{CL}$ is asymptotically Gaussian

$$G(\theta)^{1/2}(\hat{\theta}_{CL} - \theta^*) \stackrel{d}{\longrightarrow} \mathcal{N}(0, I)$$

• θ^* is the minimizer of the composite Kullback-Leibler divergence

$$CKL(\theta; g, f) = \sum_{k} E_{g} \{ \log g(\mathbf{Z} \in A_{k}) - \log f(\mathbf{Z} \in A_{k}; \theta) \} w_{k}$$

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Asymptotics III

consistency if all composite likelihood "blocks" correctly specified

$$\exists heta$$
 such that $f(\mathbf{z} \in A_k; heta) = g(\mathbf{z} \in A_k) \qquad orall k \in K$

- Space-time examples:
 - ▶ GRFs: Bevilacqua et al. (2012); Bai et al. (2012)
 - Max-stable processes: Davis et al. (2013)



Hypothesis testing

Null hypothesis H_0 : $\psi = \psi_0$ where $\theta = (\psi, \tau)$ and $\psi \in \mathbb{R}^q$

- Wald-type statistics (no invariance under reparameterization)
- Score-type statistics (numerical instability)
- Composite likelihood ratio statistics

$$W = 2\{ c\ell(\hat{ heta}_{CL}; \mathbf{z}) - c\ell(\psi_0, \hat{ au}_{CL}(\psi_0); \mathbf{z}) \}$$

Non standard distribution

$$W \xrightarrow{d} \sum_{j=1}^{q} \lambda_j \chi_{1,j}^2$$

 $\lambda_1 \ge, \ldots, \ge \lambda_q$ eigenvalues of $(H^{\psi\psi})^{-1}G_{\psi\psi}$ (Kent, 1982; Guyon, 1995)

 How to calibrate W ? Spatial example in Cattelan and Sartori (2014)



Model selection

- Model selection based on Akaike-type criterion (Takeuchi, 1976)
- composite likelihood information criterion (Varin and Vidoni, 2005)

$$CLIC = -2cl(\hat{\theta}_{CL}; \mathbf{z}) + 2 \dim(\theta)$$

• composite Bayesian information criterion (Gao and Song, 2010)

$$CBIC = -2cl(\hat{\theta}_{CL}; \mathbf{z}) + \log(n) \dim(\theta)$$

• effective number of parameters

$$\dim(\theta) = \operatorname{tr}(H(\theta)J^{-1}(\theta))$$

• CLIC has a tendency to select over-complicated models.



Model selection: example I

- 100 independent simulations from a zero mean space-time Gaussian process with covariance function C(h, u; θ)
- two space-time grids: $S \times T$, where $S = [-2, ..., 3]^2$ and $T = \{1, ..., T\}$ with T = 100, 200,
- $Z(s_i, t_i) Z(s_j, t_j) \sim \mathcal{N}(0, 2\gamma(s_i s_j, t_i t_j))$ with $\gamma(h, u) = C(0, 0; \theta) C(h, u; \theta)$
- pairwise difference likelihood

$$\mathsf{PL}(heta; \mathbf{z}) = \prod_{i>j} f(z(s_i, t_i) - z(s_j, t_j); heta)$$



Model selection: example II

model A Double exponential model (separable model)

$$C(h, u; \theta) = \sigma^2 \exp\left(-3\frac{\|h\|}{a} - 3\frac{|u|}{b}\right)$$

model B Gneiting model

$$C(h, u; \theta) = \frac{\sigma^2}{(\frac{20|u|^{2\alpha}}{b} + 1)} \exp\left\{-\frac{3\|h\|}{a(\frac{20|u|^{2\alpha}}{b} + 1)^{\beta/2}}\right\},\$$

with $\beta = 0$ (separable model) model C Gneiting model with $\beta \neq 0$;



Model selection: example III



▶ at least 70% of the models have been correctly identified.



Large data set: around 150000 observations



All that glisters is not gold...

The Merchant of Venice, W. Shakespeare

- variability matrix $J(\theta) = Var[u(\theta; \mathbf{Z})]$ key ingredient for
 - evaluating uncertainty of composite likelihood estimates
 - test statistics
 - information criteria for model selection
- the simpler case is when there are T independent replicates (in time, for instance) $\mathbf{z}(t) = (z(s_1, t), \dots, z(s_k, t))$

$$\hat{J} = \frac{1}{T} \sum_{i=1}^{T} u(\hat{\theta}_{MC}; \mathbf{z}(t)) u(\hat{\theta}_{MC}; \mathbf{z}(t))^{\top}$$

 space-time models for extreme values (Huser and Davison, 2014)



All that glisters is not gold...

The Merchant of Venice, W. Shakespeare

- more stable to estimate directly the variance matrix of θ̂_{CL} by bootstrap but computational demanding (Bags of little bootstrap ?, Kleiner et al. (2014))
- much harder when there is no replication in space or time
- analytic expressions are possible only for few special cases (spatial GRF, Bevilacqua and Gaetan (2014)) but too computational demanding $(O(n^4))$
- resampling methods based on idea of some form of "internal replication" (block-bootstrap, window subsampling)
 - difficult to specify tuning parameters (block dimension)
 - arduous with irregularly spaced temporal and spatial observations



Composite likelihood design I

- How to choose among many possible composite likelihoods?
- for example, which is preferable between
 - the pairwise marginal likelihood

$$c\ell_m(\theta; \mathbf{z}) = \sum_{i>j} w_{ij} \log f(z_i, z_j; \theta)$$

the conditional likelihood

$$c\ell_{c}(\theta; \mathbf{z}) = \sum_{i \neq j} w_{ij} \log f(z_{i}|z_{j}; \theta)$$

the pairwise difference likelihood (for GRF)

$$c\ell_d(heta; \mathbf{z}) = \sum_{i>j} w_{ij} \log f(z_i - z_j; heta)$$

- Same computational burden: $O(n^2)$
- In large settings: should all possible pairs be included?



Weighted composite likelihoods

- When efficiency is low, unequal weighting of likelihood components can be used to obtain some improvement
- Optimal weights computationally impractical
- It sensible to assume $w_{ij} = w_{ji}$ for $c\ell_m$ and $c\ell_d$

• If
$$w_{ij} = w_{ji}$$
 and $w_{ii} = 1$

$$c\ell_{c}(\theta; \mathbf{z}) = 2c\ell_{m}(\theta; \mathbf{z}) - (n-1)\sum_{i=1}^{n}\log f(z_{i}; \theta)$$

- When the marginal parameters are known, marginal and the conditional pairwise likelihood have the same efficiency.
- in space-time setting underweight observations that are far apart in time and/or space



'Simple' weighted composite likelihoods I

• weights based on the distances.

$$w_{ij}(d) = egin{cases} 1 & \|s_i - s_j\| \leq d_s, |t_i - t_j| \leq d_t, \quad d = (d_s, d_t)' \ 0 & otherwise \end{cases}$$



• Isotropy ?



'Simple' weighted composite likelihoods II

• Spatial setting results (Bevilacqua and Gaetan, 2014)



		Exponential model			Cauchy model			Wave model		
		μ	ϕ	σ^2	μ	ϕ	σ^2	μ	ϕ	σ^2
ML	bias	0.0037	-0.0015	-0.0067	0.0044	-0.0010	-0.0041	0.0012	-0.0001	-0.0022
	\mathbf{rmse}	0.0843	0.0114	0.0792	0.0973	0.0089	0.0758	0.0409	0.0027	0.0648
TAP	bias	0.0039	-0.0013	-0.0074	0.0048	-0.0015	-0.0096	0.0011	-0.0026	-0.0022
	\mathbf{rmse}	0.0851	0.0129	0.0791	0.0989	0.0094	0.0767	0.0420	0.0155	0.0675
pl_C	bias	0.0041	-0.0028	-0.0089	0.0050	-0.0034	-0.0110	0.0013	-0.0010	-0.0020
	\mathbf{rmse}	0.0900	0.0133	0.0826	0.1033	0.0120	0.0800	0.0433	0.0086	0.0691
pl_M	bias	0.0041	-0.0028	-0.0087	0.0049	-0.0034	-0.0109	0.0013	-0.0005	-0.0017
	\mathbf{rmse}	0.0901	0.0133	0.0827	0.1033	0.0120	0.0800	0.0435	0.0069	0.0694
pl_D	bias		0.0011	0.0088		-0.0004	0.0020		-0.0044	-0.0001
	\mathbf{rmse}		0.0201	0.1142		0.0120	0.0891		0.0167	0.0717



'Simple' weighted composite likelihoods III

- Practical implementation (Bevilacqua et al., 2012)
 - Get a consistent estimate for θ , $\tilde{\theta}$
 - Estimate $G(\theta, d)$ by $\hat{G}(\tilde{\theta}; d)$
 - We choose the 'lag' *d* minimizing [Ĝ(θ̃; d)]⁻¹ in the partial order of nonnegative definite matrices or equivalently

$$d^* = \operatorname*{argmin}_{d \in \mathcal{D}} \operatorname{tr}[\hat{G}(ilde{ heta}; d)]^{-1}$$

where $\ensuremath{\mathcal{D}}$ is a set of space-time lags.

Maximize

$$c\ell_m(\theta; \mathbf{z}) = \sum_{i>j} w_{ij}(d^*) \log f(z_i, z_j; \theta)$$



Joint composite estimating functions I

- First partition $R = \{(s_1, t_1), \dots, (s_n, t_n)\}$ into three subsets
 - ▶ R_S with pairs $(s_i, t_i), (s_j, t_j), i \neq j$ differing only in locations i.e. $s_i \neq s_j$, and $t_i = t_j$
 - ▶ R_T with pairs differing only in time i.e. $s_i = s_j$, and $t_i \neq t_j$
 - ▶ R_C with pairs (cross-pairs) differing in time and in space i.e. $s_i \neq s_j$, and $t_i \neq t_j$



(a) spatial pair, (b) temporal pair, (c) the spatiotemporal cross-pair



Joint composite estimating functions II • Define $c\ell_A(\theta; \mathbf{z}) = \sum_{(i,j)\in A} w_{ij} \log f(z_i, z_j; \theta)$ we have $c\ell_m(\theta; \mathbf{z}) = c\ell_S(\theta; \mathbf{z}) + c\ell_T(\theta; \mathbf{z}) + c\ell_C(\theta; \mathbf{z})$ complete = space + time + space-time

• Composite likelihood estimate $\hat{\theta}_{CL}$ solve the estimating equation

$$u(\theta; \mathbf{z}) = 0$$

$$u_{S}(\theta; \mathbf{z}) + u_{T}(\theta; \mathbf{z}) + u_{C}(\theta; \mathbf{z}) = 0$$



Joint composite estimating functions III

- Instead stack the subset composite score functions into the vector $g(\theta, \mathbf{z}) = (u_S(\theta; \mathbf{z}), u_S(\theta; \mathbf{z}), u_C(\theta; \mathbf{z}))$
- weighted quadratic objective function (looks like GMM (Hansen, 1982))

$$Q(heta; \mathbf{z}) = g(heta, \mathbf{z})^{ op} W(heta) g(heta, \mathbf{z})$$

where
$$W(\theta) = DVar[g(\theta, \mathbf{Z})]D$$
 and
 $D = diag(\sqrt{|R_S|}, \sqrt{|R_T|}, \sqrt{|R_C|}) \otimes I$ (adjustement for
different size)

• the joint composite estimating function (JCEF) estimator (Bai et al., 2012)

$$\hat{\theta}_{JCEF} = \operatorname{argmax}_{\theta} Q(\theta; \mathbf{z})$$



Joint composite estimating functions IV

- More efficient than 'simple' weighted composite likelihood for a fixed \boldsymbol{d}
- More computational demanding
 - Require at each time an evaluation of $Var[g(\theta, \mathbf{Z})]$
 - Var[g(θ, Z)] can be derived analytically for GRF, given the large number of possible pairs, computing it on the basis of analytic formulae is not practically feasible.
 - estimation of this matrix is typically achieved by subsampling techniques
- Model selection and hypothesis testing ?



Big data: block composite likelihoods I

- Estimation and prediction for spatial data (Eidsvik et al., 2014)
- A framework that allows parallel computing
- Similar approaches: Vecchia (1988); Stein et al. (2004); Caragea and Smith (2006).
- Partition a region D into M blocks D_1, \ldots, D_M , denote $\mathbf{z}_{D_k} = \{z_i, i \in D_k\}$
- Provide that the number of locations in D_k ∪ D_l is no so large for evaluating f(z_{D_k}, z_{D_l}; θ)...

$$c\ell_B(\theta; \mathbf{z}) = \sum_{l>k} \log f(\mathbf{z}_{D_k}, \mathbf{z}_{D_l}; \theta)$$

(log) block composite likelihood (pairwise composite block-likelihood)



Big data: block composite likelihoods II

- for M = 1 or M = 2 full likelihood, M = n pairwise likelihood
- *M*: trade-off between computational and statistical efficiency.
- N_k the neighbors of block k, $N_k^{
 ightarrow} = \{l > k\} \cap \{l \in N_k\}$

$$c\ell_B(heta; \mathbf{z}) = \sum_{k=1}^{M-1} \sum_{l \in N_k^{
ightarrow}} \log f(\mathbf{z}_{D_k}, \mathbf{z}_{D_l}; heta)$$



Source: Eidsvik et al. (2014)



Big data: block composite likelihoods III

Recommendation for creating blocks

• check the spatial dependence and possible anisotropies with empirical variogram

Computational efficiency

- $n_k = c$ (fixed number of observations in a block)
- $O(c^3 M | N_k^{\rightarrow} |)$ i.e. O(n)

Concurrent approach:

- Fixed-rank kriging (Cressie and Johannesson, 2008): O(n)
- Gaussian Markov random fields (Lindgren et al., 2011): $O(n^{3/2})$ for two-dimensional spatial data and $O(n^2)$ for three spatial dimensions



Software development (in R)

- is R a convenient framework for development of composite likelihood software?
- coding in R: (block) pairwise (marginal or conditional) likelihood needs parallellizable bivariate functions in way to avoid slow loops
- Graphical processing unit
- more efficient (?) coding composite likelihoods and derived quantities in low-level languages such as Fortran or C and then call into R
- efficient numerical algorithms for low-dimension integration (for non Gaussian data)
- what is already available in R: CompRandFld package for GRF



Challenges as final remarks

- "Design" issues: which terms should be included and how they have to be combined ?
 - Preliminary analysis
- Big data: parallel inference ?
- Precise estimation of uncertainty of composite likelihood estimates
- Calibration: how to calibrate test statistics ?
- Composite likelihood in hierarchical model ?
 - Composite expectation-maximization algorithm
- Can we use composite likelihoods ideas in prediction?
 - Composite kriging ?



Thanks !

Merci !

Grazie !



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