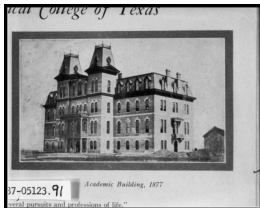


Approximate Likelihoods

Nancy Reid

November 17, 2014



Models and likelihood

- ▶ **Model** for the probability distribution of y given x
- ▶ **Density** $f(y | x)$ with respect to, e.g., Lebesgue measure
- ▶ **Parameters** for the density $f(y | x; \theta)$, $\theta = (\theta_1, \dots, \theta_d)$
- ▶ **Data** $y = (y_1, \dots, y_n)$ often independent

- ▶ **Likelihood function** $L(\theta; y) \propto f(y; \theta)$ (y_1, \dots, y_n)
- ▶ **log-likelihood function** $\ell(\theta; y) = \log L(\theta; y)$

- ▶ often $\theta = (\psi, \lambda)$

- ▶ θ could have very large dimension, $d > n$

- ▶ θ could have infinite dimension in principle
 $E(y | x) = \theta(x)$ 'smooth'

Why likelihood?

- ▶ makes probability modelling central
- ▶ emphasizes the inverse problem of reasoning from y to θ or $f(\cdot)$
- ▶ suggested by Fisher as a measure of plausibility

Royall, 1997

$L(\hat{\theta})/L(\theta) \in (1, 3)$ very plausible;

$L(\hat{\theta})/L(\theta) \in (3, 10)$ implausible;

$L(\hat{\theta})/L(\theta) \in (10, \infty)$ very implausible

- ▶ converts a 'prior' probability $\pi(\theta)$ to a posterior $\pi(\theta | y)$ via Bayes' Theorem
- ▶ provides a conventional set of summary quantities: maximum likelihood estimator, score function, ...

... why likelihood?

- ▶ likelihood function depends on data only through sufficient statistics
- ▶ “likelihood map is sufficient” Fraser & Naderi, 2007
- ▶ gives exact inference in transformation models
- ▶ “likelihood function as pivotal” Hinkley, 1980
- ▶ provides summary statistics with known limiting distribution
- ▶ leading to approximate pivotal functions, based on normal distribution
- ▶ likelihood function + sample space derivative gives better approximate inference
- ▶ basis for comparison of models, using AIC or BIC

Complicated likelihoods

generalized linear mixed models

GLM: $y_{ij} \mid u_i \sim \exp\{y_{ij}\eta_{ij} - b(\eta_{ij}) + c(y_{ij})\}$

linear predictor: $\eta_{ij} = \mathbf{x}_{ij}^T \beta + \mathbf{z}_{ij}^T \mathbf{u}_i \quad j=1, \dots, n_i; \quad i=1, \dots, m$

random effects: $\mathbf{u}_i \sim N_k(\mathbf{0}, \Sigma)$

log-likelihood:

$$\begin{aligned} \ell(\beta, \Sigma) &= \sum_{i=1}^m \left(\mathbf{y}_i^T \mathbf{X}_i \beta - \frac{1}{2} \log |\Sigma| \right. \\ &\quad \left. + \log \int_{\mathbb{R}^k} \exp\{ \mathbf{y}_i^T \mathbf{Z}_i \mathbf{u}_i - \mathbf{1}_i^T b(\mathbf{X}_i \beta + \mathbf{Z}_i \mathbf{u}_i) - \frac{1}{2} \mathbf{u}_i^T \Sigma^{-1} \mathbf{u}_i \} d\mathbf{u}_i \right) \end{aligned}$$

Ormerod & Wand 2012

... complicated likelihoods

Poisson $f(y_t | \alpha_t; \theta) = \exp(y_t \log \mu_t - \mu_t) / y_t!$

$$\log \mu_t = \beta + \alpha_t$$

autoregression

$$\alpha_t = \phi \alpha_{t-1} + \epsilon_t, \quad \epsilon_t \sim N(0, \sigma^2), \quad |\phi| < 1, \quad \theta = (\beta, \phi, \sigma^2)$$

likelihood

$$L(\theta; y_1, \dots, y_n) = \int \left(\prod_{t=1}^n f(y_t | \alpha_t; \theta) \right) f(\alpha; \theta) d\alpha$$

$L_{approx}(\theta; y)$ via Laplace with some refinements

Davis & Yau, 2011

... complicated likelihoods

$M/G/1$ queue: exponential arrival times, general service times, single server

observations y_i : times between departures from the queue

unobserved variables V_i : arrival time of customer i

model:

- ▶ $V_1 \sim \text{Exp}(\theta_3)$
- ▶ $V_i | V_{i-1} \sim V_{i-1} + \text{Exp}(\theta_3)$
- ▶ $Y_i | X_{i-1}, V_i \sim \text{Uniform}\{\theta_1 + \max(0, V_i - X_{i-1}), \theta_2 + \max(0, V_i - X_{i-1})\}$ $X_i = \sum_{j=1}^i Y_j$ $G = U(\theta_1, \theta_2)$

Likelihood

$$L(\theta; y) = \int \cdots \int f(v_1 | \theta) \prod_{i=1}^n f(v_i | v_{i-1}, \theta) \prod_{i=1}^n f(y_i | v_i, x_{i-1}, \theta) dv_1 \cdots dv_n$$

Shestopaloff & Neal, 2013

Fearnhead & Prangle, 2012

... complicated likelihoods

multivariate extremes: example, wind speed at d locations

vector observations: $(X_{1i}, \dots, X_{di}), i = 1, \dots, n$

component-wise maxima: $Z_1, \dots, Z_d; Z_j = \max(X_{j1}, \dots, X_{jn})$

Z_j are transformed (centered and scaled)

joint distribution function:

$$\Pr(Z_1 \leq z_1, \dots, Z_d \leq z_d) = \exp\{-V(z_1, \dots, z_d)\}$$

$V(\cdot)$ can be parameterized via Gaussian process models

likelihood : need the joint derivatives of $V(\cdot)$

combinatorial explosion

Davison et al., 2012

... complicated likelihoods

Ising model:

$$f(y; \theta) = \exp\left(\sum_{(j,k) \in E} \theta_{jk} y_j y_k\right) \frac{1}{Z(\theta)}$$

observations: $y_i = \pm 1$; binary property of a node i
in a graph with K nodes

parameter: θ_{jk} measures strength of interaction between
nodes i and j

E is the set of edges between nodes

partition function: $Z(\theta) = \sum_y \exp\left(\sum_{(j,k) \in E} \theta_{jk} y_j y_k\right)$

Davison 2000 §6.2

Ravikumar et al. (2010)

Xue et al. (2012)

What's a poor statistician to do?

- ▶ simplify the likelihood
 - ▶ composite likelihood
 - ▶ variational approximation
 - ▶ Laplace approximation to integrals
- ▶ change the mode of inference
 - ▶ quasi-likelihood
 - ▶ indirect inference
- ▶ simulate
 - ▶ approximate Bayesian computation
 - ▶ MCMC

Composite likelihood

- ▶ also called pseudo-likelihood
- ▶ reduce high-dimensional dependencies by ignoring them
- ▶ for example, replace $f(y_{i1}, \dots, y_{ik}; \theta)$ by

pairwise marginal $\prod_{j < j'} f_2(y_{ij}, y_{ij'}; \theta),$ or

conditional $\prod_j f_c(y_{ij} \mid y_{\mathcal{N}(ij)}; \theta)$

- ▶ Composite likelihood function

$$CL(\theta; y) \propto \prod_{i=1}^n \prod_{j < j'} f_2(y_{ij}, y_{ij'}; \theta)$$

- ▶ Composite ML estimates are consistent, asymptotically normal, not fully efficient

Besag, 1975; Lindsay, 1988

- ▶ Likelihood

$$L(\theta; y_1, \dots, y_n) = \int \left(\prod_{t=1}^n f(y_t | \alpha_t; \theta) \right) f(\alpha; \theta) d\alpha$$

- ▶ Composite likelihood

$$CL(\theta; y_1, \dots, y_n) = \prod_{t=1}^{n-1} \int \int f(y_t | \alpha_t; \theta) f(y_{t+1} | \alpha_{t+1}; \theta) f(\alpha_t, \alpha_{t+1}; \theta) d\alpha_t d\alpha_{t+1}$$

- ▶ consecutive pairs
- ▶ Time-series asymptotic regime one vector y of increasing length
- ▶ Composite ML estimator still consistent, asymptotically normal, estimable asymptotic variance
- ▶ Efficient, relative to a Laplace-type approximation
- ▶ Surprises: AR(1), fully efficient; MA(1), poor; ARFIMA(0,d,0), ok

$$\Pr(Z_1 \leq z_1, \dots, Z_d \leq z_d) = \exp\{-V(z_1, \dots, z_d; \theta)\}$$

- ▶ pairwise composite likelihood used to compare the fits of several competing models
- ▶ model choice using “CLIC”, an analogue of AIC
$$-2 \log(\widehat{CL}) + \text{tr}(J^{-1}K)$$
- ▶ Davison et al. 2012 applied this to annual maximum rainfall at several stations near Zurich
- ▶ “fitting max-stable processes to spatial or spatio-temporal block maxima is awkward ... the use of composite likelihoods ... has become widely used” Davison & Huser

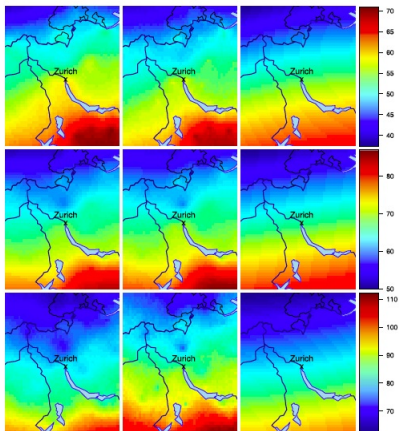


FIG. 3. Maps of the (predictive) pointwise 25-year return level estimates for rainfall (mm) obtained from the latent variable and max-stable models. The top and bottom rows show the lower and upper bounds of the 95% pointwise credible/confidence intervals. The middle row shows the predictive pointwise posterior mean and pointwise estimates. The left column corresponds to the latent variable model assuming Gamma(5, 3) prior on λ . The middle column assumes the less informative priors $\lambda_\eta \sim \text{Gamma}(1, 100)$, $\lambda_\gamma \sim \text{Gamma}(1, 10)$ and $\lambda_\delta \sim \text{Gamma}(1, 10)$. The right column corresponds to the extremal t copula model.

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Hi there!

Tell us about yourself...

Example: Ising model

Ising model:

$$f(y; \theta) = \exp\left(\sum_{(j,k) \in E} \theta_{jk} y_j y_k\right) \frac{1}{Z(\theta)}$$

neighbourhood contributions

$$f(y_j | y_{(-j)}; \theta) = \frac{\exp(2y_j \sum_{k \neq j} \theta_{jk} y_k)}{\exp(2y_j \sum_{k \neq j} \theta_{jk} y_k) + 1}$$

penalized CL estimation based on sample $y^{(1)}, \dots, y^{(n)}$

$$\max_{\theta} \left\{ \sum_{i=1}^n \ell_j(\theta; y^{(i)}) - \sum_j \sum_k P_{\lambda}(|\theta_{jk}|) \right\}$$

Xue et al., 2012

Ravikumar et al., 2010

- ▶ in a Bayesian context, want $f(\beta | y)$
use an approximation $q(\beta)$
- ▶ dependence of q on y suppressed
- ▶ choose $q(\beta)$ to be
 - ▶ simple to calculate
 - ▶ close to posterior
- ▶ simple to calculate
 - ▶ $q(\beta) = \prod q_j(\beta_j)$
 - ▶ simple parametric family
- ▶ close to posterior: minimize Kullback-Leibler divergence

$$KL(q \parallel f_{post}) = \int q(\beta) \log\{q(\beta)/f(\beta | y)\} d\beta$$

- ▶ close to posterior:

$$\min_q \int q(\beta) \log\{q(\beta)/f(\beta | y)\} d\beta = \min_q KL(q || f_{post})$$

- ▶ equivalent to

best LB for marginal $f(y)$

$$\max_q \int q(\beta) \log\{f(y, \beta)/q(\beta)\} d\beta$$

- ▶ in a likelihood context $\log f(y; \theta) = \log \int f(y | \beta; \theta) f(\beta) d\beta$

$$= \int q(\beta) \log\{f(y, \beta; \theta)/q(\beta)\} d\beta + KL(q || f_{post})$$

- ▶

$$\log f(y; \theta) \geq \int q(\beta) \log\{f(y, \beta; \theta)/q(\beta)\} d\beta$$

here β represent random effects u , or b , or ...

Example: GLMM

Ormerod & Wand, 2012

log-likelihood:

$$\begin{aligned}\ell(\beta, \Sigma) &= \sum_{i=1}^m \left(y_i^T X_i \beta - \frac{1}{2} \log |\Sigma| \right. \\ &\quad \left. + \log \int_{\mathbb{R}^k} \exp\{y_i^T Z_i u_i - 1_i^T b(X_i \beta + Z_i u_i) - \frac{1}{2} u_i^T \Sigma^{-1} u_i\} du_i \right) \\ &= \sum_{i=1}^m \left(y_i^T X_i \beta - \frac{1}{2} \log |\Sigma| \right. \\ &\quad \left. + \log \int_{\mathbb{R}^k} \exp\{y_i^T Z_i u_i - 1_i^T b(X_i \beta + Z_i u_i) - \frac{1}{2} u_i^T \Sigma^{-1} u_i\} \frac{\phi_{\Lambda_i}(u - \mu_i)}{\phi_{\Lambda_i}(u - \mu_i)} du_i \right)\end{aligned}$$

variational approx:

$$\begin{aligned}\ell(\beta, \Sigma) &\geq \sum_{i=1}^m \left(y_i^T X_i \beta - \frac{1}{2} \log |\Sigma| \right) \\ &\quad + \sum_{i=1}^m E_{u_i \sim \mathcal{N}(\mu_i, \Lambda_i)} \left(y_i^T Z_i u_i - 1_i^T b(X_i \beta + Z_i u_i) - \frac{1}{2} u_i^T \Sigma^{-1} u_i - \log\{\phi_{\Lambda_i}(u - \mu_i)\} \right) \\ &\equiv \ell(\beta, \Sigma, \mu, \Lambda) \quad \text{simplifies to } k \text{ one-dim. integrals}\end{aligned}$$



$$\ell(\beta, \Sigma) \geq \ell(\beta, \Sigma, \mu, \Lambda)$$

- ▶ **variational estimate:**

$$\ell(\tilde{\beta}, \tilde{\Sigma}, \tilde{\mu}, \tilde{\Lambda}) = \arg \max_{\beta, \Sigma, \mu, \Lambda} \ell(\tilde{\beta}, \tilde{\Sigma}, \tilde{\mu}, \tilde{\Lambda})$$

- ▶ inference for $\tilde{\beta}, \tilde{\Sigma}$? consistency? asymptotic normality?

Hall, Ormerod, Wand, 2011; Hall et al. 2011

- ▶ emphasis on algorithms and model selection

e.g. Tan & Nott, 2013, 2014

- ▶ **VL:** approx $L(\theta; y)$ by a simpler function of θ , e.g. $\prod q_j(\theta)$

- ▶ **CL:** approx $f(y; \theta)$ by a simpler function of y , e.g. $\prod f(y_j; \theta)$

Some Links between Variational Approximation and Composite Likelihoods?

S. Robin

UMR 518 AgroParisTech / INRA Applied Math & Comput. Sc.



MSTGA, Paris, November 22-23, 2012

http://carlit.toulouse.inra.fr/AIGM/pub/Reunion_nov2012/MSTGA-1211-Robin.pdf

Laplace approximation

$$\ell(\theta; y) = \log \int f(y | b; \theta)g(b)db = \log \int \exp\{Q(b, y, \theta)\}db, \text{ say}$$

$$\ell_{Lap}(\theta; y) = Q(\tilde{b}, y, \theta) - \frac{1}{2} \log |Q''(\tilde{b}, y, \theta)| + c$$

using Taylor series expansion of $Q(\cdot, y, \theta)$ about \tilde{b}

simplification of the Laplace approximation leads to PQL:

$$\ell_{PQL}(\theta, b; y) = \log f(y | b; \theta) - \frac{1}{2} b^T \Sigma^{-1} b$$

Breslow & Clayton, 1993

to be jointly maximized over b and θ

and parameters in Σ

PQL can be viewed as linearizing $E(y)$ and then using results for linear mixed models

Molenberghs & Verbeke, 2006

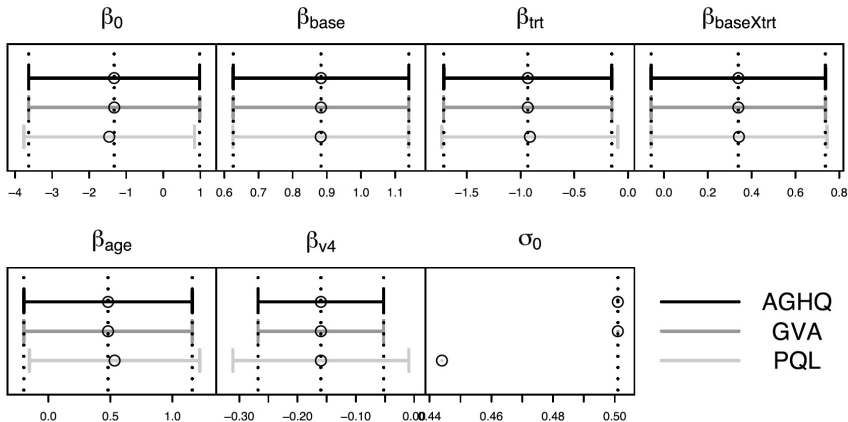


Figure 2. Point estimates and approximate 95% confidence intervals based on each of AGHQ, GVA, and PQL for the *Epilepsy* data random intercept model. The vertical dotted lines correspond to the AGHQ values.

implemented in `lme4` as `glmer`, in `MASS` as `glmmPQL`

Ormerod & Wand, 2012

Extensions of Laplace approximations

- ▶ expansions valid with $p = o(n^{1/3})$ Shun & McCullagh, 1995
- ▶ expansions for mixed linear models to higher order Raudenbush et al., 2000
- ▶ use REML for variance parameters Nelder & Lee, 1996
- ▶ integrated nested Laplace approximation Rue et al., 2009
 - ▶ model $f(y_i | \theta_i)$; prior $\pi(\theta | \vartheta)$ parameters and hyper-par
 - ▶ posterior $\pi(\theta, \vartheta | y) \propto \pi(\theta | \vartheta)\pi(\vartheta) \prod f(y_i | \theta_i)$
 - ▶ marginal posterior

$$\pi(\theta_i | y) = \int \underbrace{\pi(\theta_i | \vartheta, y)}_{\text{Laplace}} \underbrace{\pi(\vartheta | y)}_{\text{Laplace}} d\vartheta$$

Quasi-likelihood

- ▶ simplify the model



$$E(y_i; \theta) = \mu_i(\theta); \quad \text{Var}(y_i; \theta) = \phi \nu_i(\theta)$$

- ▶ consistent with generalized linear models
- ▶ example: over-dispersed Poisson responses
- ▶ PQL uses this construction, but with random effects

Molenberghs & Verbeke, Ch. 14

- ▶ why does it work?
- ▶ score equations are the same as for a 'real' likelihood

hence unbiased

- ▶ derivative of score function equal to variance function

special to GLMs

Indirect inference

- ▶ composite likelihood estimators are consistent
under conditions ...
- ▶ because $\log CL(\theta; y) = \sum_{i=1}^n \sum_{j < j'} \log f(y_j, y_{j'}; \theta)$
- ▶ derivative w.r.t. θ has expected value 0

- ▶ what happens if an estimating equation $g(y; \theta)$ is **biased**?
- ▶ $g(y_1, \dots, y_n; \tilde{\theta}_n) = 0; \quad \tilde{\theta}_n \rightarrow \theta^* \quad \text{E}g(Y; \theta^*) = 0$

- ▶ $\theta^* = \tilde{k}(\theta); \text{invertible? } \theta = k(\theta^*) \quad \tilde{k}^{-1} \equiv k$

- ▶ **new estimator** $\hat{\theta}_n = k(\tilde{\theta}_n)$
- ▶ $k(\cdot)$ is a **bridge** function, connecting wrong value of θ to the right one
Yi & R, 2010; Jiang & Turnbull, 2004

- ▶ model of interest

$$y_t = G_t(y_{t-1}, x_t, \epsilon_t; \theta), \quad \theta \in \mathbb{R}^d$$

- ▶ likelihood is not-computable, but can simulate from the model
- ▶ simple (wrong) model

$$y_t \sim f(y_t | y_{t-1}, x_t; \theta^*), \quad \theta^* \in \mathbb{R}^p$$

- ▶ find the MLE in the simple model, $\hat{\theta}^* = \hat{\theta}^*(y_1, \dots, y_n)$, say
- ▶ use simulated samples from model of interest to find the 'best' β
- ▶ 'best' θ gives data that reproduces $\hat{\theta}^*$

Shalizi, 2013

- ▶ simulate samples y_t^m , $m = 1, \dots, M$ at some value θ
- ▶ compute $\hat{\theta}^*(\theta)$ from the simulated data

$$\hat{\theta}^*(\theta) = \arg \max_{\theta^*} \sum_m \sum_t \log f(y_t^m | y_{t-1}^m, x_t; \theta^*)$$

- ▶ choose θ so that $\hat{\theta}^*(\theta)$ is as close as possible to $\hat{\theta}^*$
- ▶ if $p = d$ simply invert the ‘bridge function’
- ▶ usually $p > d$
 - ▶ $\hat{\theta}_1 = \arg \min_{\theta} \{ \hat{\theta}^*(\theta) - \hat{\theta} \}^T W \{ \hat{\theta}^*(\theta) - \hat{\theta} \}$
 - ▶ $\hat{\beta}_2 = \arg \min_{\theta} (\sum_t \log f(y_t | y_{t-1}, x_t, \hat{\theta}^*(\theta)) - \sum_t \log f(y_t | y_{t-1}, x_t, \hat{\theta}))$
- ▶ estimates of θ are consistent, asymptotically normal, but not efficient

- ▶ simulate θ' from $\pi(\theta)$
- ▶ simulate data z from $f(\cdot; \theta')$
- ▶ if $z = y$ then θ' is an observation from posterior $\pi(\cdot | y)$
- ▶ actually $s(z) = s(y)$ for some set of statistics
- ▶ actually $\rho\{s(z), s(y)\} < \epsilon$ for some distance function $\rho(\cdot)$

Fearnhead & Prangle, 2011

- ▶ many variations, using different MCMC methods to select candidate values θ'

... approximate Bayesian computation

M/G/1 queue: exponential arrival times, general service times, single server

observations y_i : times between departures from the queue

unobserved variables V_i : arrival time of customer i

model:

- ▶ $V_1 \sim \text{Exp}(\theta_3)$
- ▶ $V_i | V_{i-1} \sim V_{i-1} + \text{Exp}(\theta_3)$
- ▶ $Y_i | X_{i-1}, V_i \sim \text{Uniform}\{\theta_1 + \max(0, V_i - X_{i-1}), \theta_2 + \max(0, V_i - X_{i-1})\}$ $X_i = \sum_{j=1}^i Y_j$
- ▶ service time $\sim U(\theta_1, \theta_2)$

ABC: use quantiles of departure times as summary statistics

Indirect Inference: use \bar{y} , $y_{(1)}$, $\hat{\theta}_2$ from steady-state model

Table 7. Mean quadratic losses for various analyses of 50 $M/G/1$ data sets[†]

<i>Method</i>	θ_1	θ_2	θ_3
Comparison	1.1	2.2	0.0013
Comparison + regression	<i>0.020</i>	1.1	<i>0.0013</i>
Semi-automatic ABC	<i>0.022</i>	1.0	<i>0.0013</i>
Semi-automatic predictors	0.024	1.2	0.0017
Indirect inference	0.18	<i>0.42</i>	0.0033

[†]Losses within 10% of the smallest values for that parameter are italicized.

- ▶ both methods need a set of parameter values from which to simulate: θ' or θ
- ▶ both methods need a set of auxiliary functions of the data $s(y)$ or $\hat{\theta}^*(y)$
- ▶ in indirect inference, $\hat{\theta}^*$ is the 'bridge' to the parameters of real interest, θ
- ▶ C & K use orthogonal designs based on Hadamard matrices to chose θ'
- ▶ and calculate summary statistics focussed on individual components of θ
- ▶ MCMC estimation of log-likelihood function

Geyer & Thompson, 1992

cond. comp. likelihood poor for Ising model

Okabayashi et al., 2011

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FIELDS

THEMATIC PROGRAM ON STATISTICAL INFERENCE, LEARNING, AND MODELS FOR

JANUARY - JUNE, 2015

PROGRAM

JANUARY 12 – 23, 2015

Opening Conference and Boot Camp

Organizing Committee: Nancy Reid (Chair), Sallie Keller, Lisa Lix, Bin Yu

JANUARY 26 – 30, 2015

Workshop on Big Data and Statistical Machine Learning

Organizing committee: Ruslan Salakhutdinov (Chair), Dale Schuurmans, Yoshua Bengio, Hugh Chipman, Bin Yu

FEBRUARY 9 – 13, 2015

Workshop on Optimization and Matrix Methods in Big Data

Organizing Committee: Stephen Vavasis (Chair), Anima Anandkumar, Petros Drineas, Michael Friedlander, Nancy Reid, Martin Wainwright

FEBRUARY 23 – 27, 2015

Workshop on Visualization for Big Data: Strategies and Principles

Organizing Committee: Nancy Reid (Chair), Susan Holmes, Snehelata Huzurbazar, Hadley Wickham, Leland Wilkinson

MARCH 23 – 27, 2015

Workshop on Big Data in Health Policy

Organizing Committee: Lisa Lix (Chair), Constantine Gatsonis, Sharon-Lise Normand

APRIL 13 – 17, 2015

Workshop on Big Data for Social Policy

BIG DATA

This thematic program emphasizes both applied and theoretical aspects of statistical inference, learning and models in big data. The opening conference will serve as an introduction to the program, concentrating on overview lectures and background preparation. Workshops throughout the program will highlight cross-cutting themes, such as learning and visualization, as well as focus themes for applications in the social, physical and life sciences. It is expected that all activities will be webcast using the FieldsLive system to permit wide participation. Allied activities planned include workshops at PIMS in April and May and CRM in May and August.

ORGANIZING COMMITTEE

Yoshua Bengio (Montréal)

Hugh Chipman (Acadia)

Sallie Keller (Virginia Tech)