Bayesian model configuration, selection and averaging in complex regression contexts

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1. Introduction;

- 2. The Deep Bayesian regression model (DBRM)
 - Feature engineering;
 - Bayesian model specification
 - Links to GLM(M)s and logic regressions;
- 3. (R)(G)MJMCMC algorithm
- 4. Applications
 - Prediction:
 - Inference.

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Complex regression models

Mapping explanatory variables X to the responses Y via $Y \sim F(X, \theta)$. **Purposes:**

- 1. Inference:
 - Explain how and why X influences Y.
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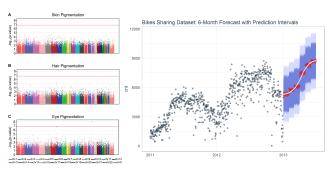


Figure: Prediction and inference illustrations

1. Regression problems:

- Prediction of house prices;
- Explaining which factors influence the amount of rainfall.
- 2. Classification problems
 - Classify objects from the pictures;
 - Explain why a particular person is rejected a mortgage.
- 3. Ranking problems
 - Rank a set of articles w.r.t. their relevance to a given person;
 - Identify which factors cause a particular SP Rating of a country.
- 4. Time to event problems
 - Predict how likely an insurance event will happen within a given horizon:
 - Identify which factors increase the probability of survival of a patient within a given horizon.

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Models

1. Linear:

- Linear regression (LR);
- Generalized linear model (GLM);
- Mixed linear models (LMM, GLMM);
- Gaussian processes (GP);
- Support vector machines, etc.

Nonlinear

- Classification and regression trees (CART);
- Generalized additive models (GAM);
- Generalized additive mixed models (GAMM);
- Deep Gaussian processes (DGP)
- Artificial neural netweorks (ANN), etc.



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Problems and goals

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- 1. Models for inference and predictions do not coincide;
- 2. Manual selection of an optimal model and a set of explanatory variables from a huge set of possibilities is hard and requires strong statistical expertise.

Main aims

- 1. Develop automatic model selection and configuration for both good inference and predictions;
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1. Consider a class of models $\Omega: m_1(Y|X, \theta_1), ..., m_k(Y|X, \theta_k)$;

- 2. Put priors for all models $p(m_1),...,p(m_k)$ and their parameters $p(\theta_1|m_1),...,p(\theta_k|m_k)$;
- 3. Obtain the joint posterior distribution of models and parameters $p(m_1, \theta_1|D), ..., p(m_k, \theta_k|D)$;
- 4. Make inference on Δ in the joint space of models and parameters: $p(\Delta|D) = \int_{\Omega} p(m|D) \int_{\Theta} p(\Delta|m,\theta,D) p(\theta|m,D) d\theta dm;$
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Deep Bayesian Regression Model, Paper III

Sample of observations $i = 1, \dots, n$

- Y_i . . . response data;
- $x_i = (x_{i1}, \dots, x_{ip}) \dots p$ -dimensional vector of input covariates.

Specification of the mode

From input variables a huge (but finite) number of features can be generated: $F_j(x_i)$, j=1,...,q (consider ordering w.r.t. complexity) The model is then specified as GLM:

$$Y_i|\mu_i, \phi \sim f(y|\mu_i, \phi), i = 1, ..., n;$$
 (1)

$$h(\mu_i) = \beta_0 + \sum_{j=1}^q \gamma_j \beta_j F_j(\mathbf{x}_i) . \tag{2}$$

- f(·|μ, φ) density from exponential family with mean μ_i and dispersion parameter φ;
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$$F_j(\mathbf{x}) = \begin{cases} v(F_k(\mathbf{x})), & \text{for a modification;} \\ F_k(\mathbf{x}) * F_l(\mathbf{x}), & \text{for a crossover;} \\ v(\boldsymbol{\alpha}^T \mathbf{F}(\mathbf{x})), & \text{for a projection;} \end{cases}$$

- $F_k(\mathbf{x})$ and $F_l(\mathbf{x})$ are previously defined features (k, l < j);
- $v \in \mathcal{G}$ is one of the allowed basic function from set \mathcal{G} ;
- $\mathbf{F}(\mathbf{x})$ is a sub-vector of all possible features with indexes 1, ..., j-1;
- A constraint on the complexity of feature $F_j(\mathbf{x})$ is defined by a finite number q of all possible features;
- Projections include modifications and crossovers as particular cases

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Other remarks

Types and meaning of functions in ${\cal G}$

- Neural Networks: logit(x), tanh(x), erf(x), ReLU(x);
- Polynomials: $F_k(\mathbf{x}) * F_l(\mathbf{x}) = \exp(\log(F_k(\mathbf{x})) + \log(F_l(\mathbf{x})))$;
- CART: $I(x \ge 1)$;
- MARS: $\max\{0, x t\}$ and $\max\{0, t x\}$;
- Fractional polynomials: $x^{\frac{1}{a}} = \exp(b \log(x)), b = \frac{1}{a}$;
- Logical AND, OR and NOT: $L_k \wedge L_l = L_k * L_l$, $L_k \vee L_l = L_k + L_l L_k * L_l$, and $\overline{L}_k = 1 L_k$.

Potential extension of DBRN

Include Gaussian latent variables $\delta_{k} = (\delta_{1k}, ..., \delta_{nk}) \sim N_{n}(\mathbf{0}, \mathbf{\Sigma}_{k})$ to model correlation structure or overdispersion for GLM

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- Polynomials: $F_k(\mathbf{x}) * F_l(\mathbf{x}) = \exp(\log(F_k(\mathbf{x})) + \log(F_l(\mathbf{x})))$;
- CART: $I(x \ge 1)$;
- MARS: $\max\{0, x t\}$ and $\max\{0, t x\}$;
- Fractional polynomials: $x^{\frac{1}{a}} = \exp(b \log(x)), b = \frac{1}{a}$;
- Logical AND, OR and NOT: $L_k \wedge L_l = L_k * L_l$, $L_k \vee L_l = L_k + L_l L_k * L_l$, and $\overline{L}_k = 1 L_k$.

Potential extension of DBRM

$$h(\mu_i) = \beta_0 + \sum_{i=1}^q \gamma_j \beta_j F_j(\mathbf{x}_i) + \sum_{k=1}^r \lambda_k \delta_{ik}.$$

Prior specification

Model priors

Model topology defined by $\mathfrak{m} = (\gamma_1, \dots, \gamma_q)$ Priors of \mathfrak{m} should guarantee regularization (parsimonious models)

$$p(\mathfrak{m}) \propto \mathsf{I}(|\gamma_{1:q}| \leq Q) \prod_{j=1}^{q} a^{\gamma_j c(F_j(\mathsf{x}))}, \quad 0 < a < 1$$
 (3)

- $c(F_j(\mathbf{x})) \ge 0$ non-decreasing **complexity measure** of feature $F_j(\mathbf{x})$;
- Q is the maximal number of features per given model.

Example: Total width (sum of width of all nested features involved); GLMM: boils down to a simple prior $p(\mathfrak{m}) \propto \prod_{j=1}^q a^{\gamma_j}$; BLR: $a^{c(L_j)} = \frac{1}{N(s_i)}$, $s_j \leq C_{max}$, $N(s_j)$ - number of trees with s_j leaves

Parameter priors

Priors for β_j (and ϕ): Problem-specific and computational considerations \Rightarrow Conjugate priors, Jeffrey's priors, robust g priors, etc.

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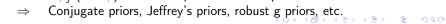
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Marginal likelihood $P(D|\mathfrak{m}) = \int_{\theta_{\mathfrak{m}} \in \Theta_{\mathfrak{m}}} p(D|\theta_{\mathfrak{m}},\mathfrak{m}) p(\theta_{\mathfrak{m}}|\mathfrak{m}) d\theta_{\mathfrak{m}}$ Conjugate priors, Laplace approximation, INLA, Variational inference, etc.

$$P(\mathfrak{m}|D) = \frac{P(D|\mathfrak{m})p(\mathfrak{m})}{\sum_{\mathfrak{m}' \in \Omega} P(D|\mathfrak{m}')p(\mathfrak{m}')} , \qquad (4)$$

Denominator

- Classical MCMC: use relative frequency of models in Markov chain;
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$$P(\mathfrak{m}|D) \approx \frac{P(D|\mathfrak{m})P(\mathfrak{m})}{\sum_{\mathfrak{m}' \in \Omega^*} P(D|\mathfrak{m}')P(\mathfrak{m}')} \quad \text{for} \quad \mathfrak{m} \in \Omega^*.$$
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Hubin and Storvik (2018)

Variable selection with p potential exploratory variables

- 2^p potential models;
- Multimodality ⇒ MCMC trapped by local maxima or extremely low acceptance ratio.

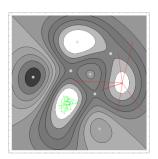


Figure: MCMC with either small (green) or large (red) proposals



Mode jumping MCMC (MJMCMC)

- After certain number of MCMC steps make a jump
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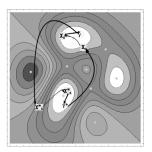


Figure: Locally optimized with randomization proposals

The protein activity data. 288 models. Multiple modes

Comparison to other algorithms. On 2^{20} unique models visited for MJMCMC, ESS and BAS and 88×2^{20} iterations of RS.

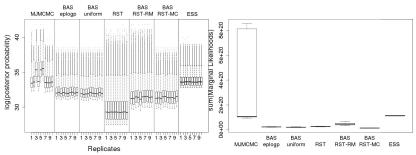


Figure: 100000 best mliks found (left) and posterior masses captured (right). Bayesian linear regression with a g-prior is addressed

Problem for DBRM (Logic Regressions)

- Diffcult to fully specify the model space Ω ;
- Also q too large for MJMCMC.

- MJMCMC is embedded in a genetic algorithm which updates a finite population of features of size $d \ll q$;
- Populations $\mathcal{S}_1, \mathcal{S}_2, ..., \mathcal{S}_{\mathcal{T}_{max}} \quad \Rightarrow \quad \text{each } \mathcal{S}_t \text{ is a set of } d \text{ features;}$
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- Otherwise a transition $\mathfrak{m} \to \mathfrak{m}^* \to \mathfrak{m}^1 \to ... \to \mathfrak{m}^k \to \mathfrak{m}'$ is considered with a given probability kernel:
 - q(m*|m) is the proposal for the solution in the new search space induced by S':
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 - Transition m^{*} → m['] is some randomization at the end of the procedure;
- Acceptance probability for such a procedure is $r_m = \min\{1, \alpha_m\}$

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Parallelization

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A memory efficient alternative is:

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Comparison of algorithms

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 - DBRM_G and DBRM_G_PAR: Using GMJMCMC with 1 or 32 threads;
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Three binary classification tasks (Deep logistic regression)

- Asteroids data: Mean anomaly, Inclination, Argument of perihelion, Longitude of the ascending node, Rms residual, Semi major axis, Eccentricity, Mean motion, Absolute magnitude;
- Breast cancer data: Radius, texture, perimeter, area, smoothness, compactness, concavity, concave points, symmetry, fractal dimension;
- Spam emails: 58 characteristics, including 57 continuous and 1 nominal variable, where most of these are concerned with the frequency of particular words or characters. 3 provide different measurements on the sequence length of consecutive capital letters.

- Accuracy of predictions (ACC);
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Deep Bayesian logsitic regression

$$y_i = y | \rho_i \sim \mathsf{Binom}(1, \rho_i);$$
 (9)

$$\rho_{i} = \frac{e^{\gamma_{\mathbf{0}}\beta_{\mathbf{0}} + \sum_{j=1}^{q} \gamma_{j}\beta_{j}F_{j}(\mathbf{x}_{i})}}{1 + e^{\gamma_{\mathbf{0}}\beta_{\mathbf{0}} + \sum_{j=1}^{q} \gamma_{j}\beta_{j}F_{j}(\mathbf{x}_{i})}};$$
(10)

$$p(\gamma) \propto I(|\gamma_{1:q}| \leq 20) \prod_{j=1}^{q} \exp(-\gamma_j 2c(F_j(x))); \tag{11}$$

$$p(\beta|\gamma) = |J_n^{\gamma}(\beta)|^{\frac{1}{2}}; \tag{12}$$

$$G = \{ sigmoid(x), I(x > 1), ReLu(x), x^{\frac{1}{3}}, x^{\frac{1}{5}} \}.$$
 (13)

Example 1

Asteroid classification

Training sample: n = 64, Test sample: $n_p = 20702$

Algorithm	ACC	FNR	FPR
LBRM	0.9999 (0.9999,0.9999)	0.0001	0.0002
DBRM_G_PAR	0.9998 (0.9986,1.0000)	0.0002	0.0000
DBRM_R_PAR	0.9998 (0.9964,0.9999)	0.0002	0.0000
DBRM_R	0.9998 (0.9946,1.0000)	0.0002	0.0002
DBRM_G	0.9998 (0.9942,1.0000)	0.0002	0.0002
LASSO	0.9991 (-,-)	0.0013	0.0000
RIDGE	0.9982 (-,-)	0.0026	0.0000
LXGBOOST	0.9980 (0.9980,0.9980)	0.0029	0.0000
LR	0.9963 (-,-)	0.0054	0.0000
DEEPNETS	0.9728 (0.8979,0.9979)	0.0384	0.0000
TXGBOOST	0.8283 (0.8283,0.8283)	0.0005	0.3488
RFOREST	0.8150 (0.6761,0.9991)	0.1972	0.0162
NBAYES	0.6471 (-,-)	0.0471	0.4996



Example 2

Breast cancer data

Training sample: n = 142, Test sample: $n_p = 427$

Algorithm	ACC	FNR	FPR
DBRM_R_PAR	0.9765 (0.9695,0.9812)	0.0479	0.0074
DBRM_G_PAR	0.9742 (0.9695,0.9812)	0.0479	0.0111
RIDGE	0.9742 (-,-)	0.0592	0.0037
LBRM	0.9718 (0.9648,0.9765)	0.0592	0.0074
DBRM_G	0.9695 (0.9554,0.9789)	0.0536	0.0148
DEEPNETS	0.9695 (0.9225,0.9789)	0.0674	0.0074
DBRM_R	0.9671 (0.9577,0.9812)	0.0536	0.0148
LR	0.9671 (-,-)	0.0479	0.0220
LASSO	0.9577 (-,-)	0.0756	0.0184
LXGBOOST	0.9554 (0.9554,0.9554)	0.0809	0.0184
TXGBOOST	0.9531 (0.9484,0.9601)	0.0647	0.0326
RFOREST	0.9343 (0.9038,0.9624)	0.0914	0.0361
NBAYES	0.9272 (-,-)	0.0305	0.0887



Example 3

Spam data

Training sample: n = 1536, Test sample: $n_p = 3065$

Algorithm	ACC	FNR	FPR
TXGBOOST	0.9465 (0.9442,0.9481)	0.0783	0.0320
RFOREST	0.9328 (0.9210,0.9413)	0.0814	0.0484
DEEPNETS	0.9292 (0.9002,0.9357)	0.0846	0.0531
DBRM_R_PAR	0.9268 (0.9162,0.9390)	0.0897	0.0538
DBRM_G_PAR	0.9251 (0.9139,0.9377)	0.0897	0.0552
DBRM_G	0.9243 (0.9113,0.9328)	0.0927	0.0552
DBRM_R	0.9237 (0.9106,0.9351)	0.0917	0.0557
LR	0.9194 (-,-)	0.0681	0.0788
LBRM	0.9178 (0.9168,0.9188)	0.1090	0.0528
LASSO	0.9171 (-,-)	0.1077	0.0548
RIDGE	0.9152 (-,-)	0.1288	0.0415
LXGBOOST	0.9139 (0.9139,0.9139)	0.1083	0.0591
NBAYES	0.7811 (-,-)	0.0801	0.2342

Example1:	Asteroid						
complexity	G	R	G_PAR	R_PAR	LBRM		
1	8.96	8.97	9.00	9.00	9.00		
2	2.58	2.62	0.05	0.15	0.00		
Total	11.54	11.59	9.05	9.15	9.00		
Example2: Breast cancer							
complexity	G	R	G PAR	R PAR	LBRM		

Example 2 : Breast cancer						
complexity	G	R	G_PAR	R_PAR	LBRM	
1	11.30	11.73	14.20	10.79	29.83	
2	3.09	3.06	0.04	0.21	0.00	
3	0.30	0.00	0.00	0.00	0.00	
6	0.00	0.01	0.00	0.00	0.00	
7	0.00	0.01	0.00	0.00	0.00	

• Non-linear features don't play an important role;

14.81

• Still DBRM performs very well ⇒ not too much overfitting;

14.24

11.00

29.83

• Parallel version much better performance.

14.42

Total



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Evample 3: Snam mail

Examples:	Spam ma	II			
complexity	G	R	G_PAR	R_PAR	LBRM
1	36.34	36.09	39.87	39.17	49.83
2	14.45	14.83	21.47	22.43	0.00
3	2.83	3.17	5.24	5.81	0.00
4	0.69	0.57	1.36	1.36	0.00
5	1.15	1.09	1.56	1.68	0.00
6	0.92	0.74	1.24	1.07	0.00
7	0.37	0.40	0.57	0.42	0.00
8	0.25	0.22	0.33	0.17	0.00
9	0.04	0.08	0.16	0.11	0.00
≥10	0.15	0.11	0.11	0.18	0.00
Total	57.190	57.300	71.910	72.400	49.830

- Non-linear features are important for spam filter;



Example3: Spam mail

Examples.	Spain ma	II			
complexity	G	_ R	G_PAR	R_PAR	LBRM
1	36.34	36.09	39.87	39.17	49.83
2	14.45	14.83	21.47	22.43	0.00
3	2.83	3.17	5.24	5.81	0.00
4	0.69	0.57	1.36	1.36	0.00
5	1.15	1.09	1.56	1.68	0.00
6	0.92	0.74	1.24	1.07	0.00
7	0.37	0.40	0.57	0.42	0.00
8	0.25	0.22	0.33	0.17	0.00
9	0.04	0.08	0.16	0.11	0.00
≥10	0.15	0.11	0.11	0.18	0.00
Total	57.190	57.300	71.910	72.400	49.830

- Non-linear features are important for spam filter;
- Parallel version gives here more complex features;
- Interpretability: Certain non-linear features appear quite reproducible by DBRM over 100 independent runs.



Example3: Spam mail

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complexity	G	_ R	G_PAR	R_PAR	LBRM
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2	14.45	14.83	21.47	22.43	0.00
3	2.83	3.17	5.24	5.81	0.00
4	0.69	0.57	1.36	1.36	0.00
5	1.15	1.09	1.56	1.68	0.00
6	0.92	0.74	1.24	1.07	0.00
7	0.37	0.40	0.57	0.42	0.00
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Deep Gaussian regression model

Dataset: Ten physical parameters of n = 223 exoplanets. We want to recover 2 basic physical laws.

Input variables include: Mean anomaly, Inclination, Argument of perihelion, Longitude of the ascending node, Rms residual, Semi major axis, Eccentricity, Mean motion, Absolute magnitude.

Example 4: Planetary mass

$$m_p \approx K_1 R_p^3 \times \rho_p$$

Planetary mass m_p is proportional to cube of radius R_p times the density of the planet ρ_p

Example 5: Kepler's third law

The square of the orbital period P of a planet is directly proportional to the cube of the semi-major axis a of its orbit:

$$a \approx K_2 \left(P^2 M_h \right)^{\frac{1}{3}}$$

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Deep Bayesian Gaussian regression

$$Y_i|\mu_i,\sigma^2 \sim N(\mu_i,\sigma^2), i \in \{1,...,n\};$$
 (14)

$$\mu_i = \gamma_0 \beta_0 + \sum_{j=1}^q \gamma_j \beta_j F_j(\mathbf{x}_i); \tag{15}$$

$$p(\gamma) \propto |(|\gamma_{1:q}| \leq 15) \prod_{j=1}^{q} \exp(-2\log n\gamma_j c(F_j(x)));$$
 (16)

$$p(\beta|\gamma) = |J_n^{\gamma}(\beta)|^{\frac{1}{2}}; \tag{17}$$

$$\pi(\sigma^2) = \sigma^{-2};\tag{18}$$

$$\mathcal{G} = \{ \operatorname{sigmoid}(x), \cos(x), \tanh(x), \operatorname{atan}(x), |x|^{\frac{1}{3}} \}.$$
 (19)

- Example 4: only feature $R_p^3 \times \rho_p$ counted as true positive (TP);
- Example 5: $(P^2M_h)^{\frac{1}{3}}$, $(P^2T_h)^{\frac{1}{3}}$, $(P^2FE_h)^{\frac{1}{3}}$ counted as TP;
- Power, FDR and average number of false positives (FP) estimated by 100 runs of DBRM;
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- Different numbers of parallel runs

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- Different numbers of parallel runs.

	DBRM_G_PAR			DBRM_R_PAR			
Threads	Power	FP	FDR	Power	FP	FDR	
16	1.00	0.00	0.00	0.97	0.06	0.03	
4	0.79	0.40	0.21	0.61	0.73	0.39	
1	0.42	1.21	0.58	0.33	1.63	0.67	

- Power increases with number of parallel threads;
- FP and FDR decrease with number of parallel threads;
- GMJMCMC slightly better than RGMJMCMC.

	DBRI	$M_{G_{G}}$	PAR	DBRM_R_PAR			
Threads	Power	FP	FDR	Power	FP	FDR	
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4	0.79	0.40	0.21	0.61	0.73	0.39	
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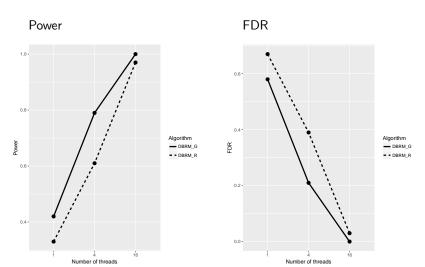
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	DBRM_G_PAR						DBRM_R_PAR					
Thr	F_1	F_2	F_3	Pow	FP	FDR	F_1	F_2	F_3	Pow	FP	FDR
					0.02							
16	34	41	32	0.84	0.46	0.18	31	38	18	0.79	0.68	0.25
1	6	5	3	0.14	0.65	0.86	6	4	2	0.12	1.81	0.88

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	DBRM_G_PAR						DBRM_R_PAR					
Thr	F_1	F_2	F_3	Pow	FP	FDR	F_1	F_2	F_3	Pow	FP	FDR
64	81	71	1	1.00	0.02	0.01	78	75	2	0.99	0.03	0.01
16	34	41	32	0.84	0.46	0.18	31	38	18	0.79	0.68	0.25
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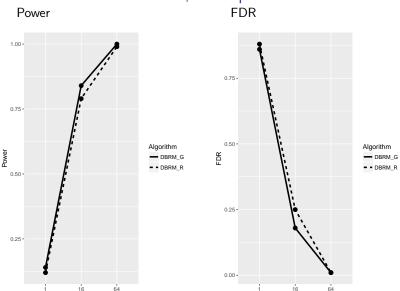
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Results, Example 5



Number of threads



Number of threads

Bayesian logic regression domain

For Example 6 we generated N=100 datasets with n=1000 observations and p=50 binary covariates. The covariates were assumed to be independent and were simulated as $X_j \sim \text{Bernoulli}(0.5)$ for $j \in \{1, \dots, 50\}$.

Continuous responses

Gaussian observations with error variance $\sigma^2=1$ and individual expectations specified as follows for the different scenarios:

Example 6

$$E(Y|X) = 1 + 1.5 X_7 + 1.5 X_8 + 6.6 X_{18} \land X_{21} + 3.5 X_2 \land X_9 + 9 X_{12} \land X_{20} \land X_{37} + 7 X_1 \land X_3 \land X_{27} + 7 X_4 \land X_{10} \land X_{17} \land X_{30} + 7 X_{11} \land X_{13} \land X_{19} \land X_{50}.$$

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Table: Examples 6. Inference. 32 Threads

	GMJ	RGMJ	GMJ(logic)
- X ₇	1.0000	1.0000	0.9900
X_8	1.0000	1.0000	1.0000
$X_2 \wedge X_9$	1.0000	0.9600	1.0000
$X_{18} \wedge X_{21}$	1.0000	1.0000	0.9600
$X_1 \wedge X_3 \wedge X_{27}$	1.0000	1.0000	1.0000
$X_{12} \wedge X_{20} \wedge X_{37}$	1.0000	1.0000	0.9900
$X_4 \wedge X_{10} \wedge X_{17} \wedge X_{30}$	0.9900	0.9200	0.9100
$X_{11} \wedge X_{13} \wedge X_{19} \wedge X_{50}$	0.9800	0.8900	0.3800
Overall Power	0.9963	0.9712	0.9038
FP	0.5100	1.1400	1.0900
FDP	0.0601	0.1279	0.1310

- Power is the best for DBRM with GMJMCMC;
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Concluding remarks

- We introduced the (R)(G)MJMCMC algorithm for various regresson contexts capable of:
 - Performing model configuration;
 - Estimating posterior model probabilities;
 - Bayesian model averaging and selection.
- EMJMCMC R-package is available:
 - http://aliaksah.github.io/EMJMCMC2016/;
 - Flexibility in the choice of methods for:
 - Marginal likelihoods;
 - Model selection criteria;
 - Extensive parallel computing is available;
 - Vectorized predictions with NA handling is incorporated.
- Results showed that (R)(G)MJMCMC:
 - Performs well in terms of the search speed and quality;
 - Provides nice predictive and inferential performance in the applications.



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