Bayesian computing with INLA

King Abdullah University of Science and Technology



Håvard Rue King Abdullah University of Science and Technology Saudi-Arabia

Oct 2018

∃ ▶ ∢ ∃ ▶



- INLA do approximate Bayesian inference for a spesific class of models
- This is the class of latent Gaussian models
- In most cases, INLA is faster and more accurate inference than with MCMC
- Cannot do *all models*, then the ones we can do, we do very very well.
- Many/most of the important models that people use, we can do





- INLA do approximate Bayesian inference for a spesific class of models
- This is the class of latent Gaussian models
- In most cases, INLA is faster and more accurate inference than with MCMC
- Cannot do *all models*, then the ones we can do, we do very very well.
- Many/most of the important models that people use, we can do





- INLA do approximate Bayesian inference for a spesific class of models
- This is the class of latent Gaussian models
- In most cases, INLA is faster and more accurate inference than with MCMC
- Cannot do *all models*, then the ones we can do, we do very very well.
- Many/most of the important models that people use, we can do



Oct 2018 2 / 135



- INLA do approximate Bayesian inference for a spesific class of models
- This is the class of latent Gaussian models
- In most cases, INLA is faster and more accurate inference than with MCMC
- Cannot do *all models*, then the ones we can do, we do very very well.
- Many/most of the important models that people use, we can do



Oct 2018 2 / 135

- NEVER MIND THE BIG DATA HERE'S THE BIG NOCES
- INLA do approximate Bayesian inference for a spesific class of models
- This is the class of latent Gaussian models
- In most cases, INLA is faster and more accurate inference than with MCMC
- Cannot do *all models*, then the ones we can do, we do very very well.
- Many/most of the important models that people use, we can do



www.r-inla.org





Oct 2018 3 / 135

・ロト ・聞 ト ・ ヨト ・ ヨト

Books





Oct 2018 4 / 135

◆□▶ ◆□▶ ◆□▶ ◆□▶

Books, and more to come...





ADVANCED SPATIAL MODELING WITH STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS USING R AND INLA



ELIAS T. KRAINSKI VIRGILIO GÓMEZ-RUBIO HAAKON BAKKA AMANDA LENZI DANIELA CASTRO-CAMILO DANIEL SIMPSON FINN LINDGREN HÅVARD RUE

> CRC Press Taylor & Francis Group A CHAPMAN & HALL BOC

A B > A B > A B >
 A
 B >
 A
 B >
 A
 B >
 A
 B >
 A
 B >
 A
 B >
 A
 B >
 A
 B >
 A
 B >
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 B
 A
 A
 A

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 5 / 135



EFFICIENT RECONSTRUCTIONS OF COMMON ERA CLIMATE VIA INTEGRATED NESTED LAPLACE APPROXIMATIONS.

LUIS A. BARBOZA, JULIEN EMILE-GEAY, BO LI, AND WAN HE

ABSTRACT. A Paleoclimate Reconstruction on the Common Era (1-2000AD) was performed using a Hierarchical Bayesian Model from three types of data: proxy data from PAGES2k project dataset, HadCRUT4 temperature data from the Climatic Research Unit at the University of East Anglia, and external forcing data from several sources. Five data reduction techniques were explored with the purpose of achieving a parsimoneous but sufficient set of proxy equations. Instead of using the MCMC approach to solve for the latent variable, we employed an INLA algorithm that can approximate the MCMC results and meantime is much more computationally efficient than MCMC. The role of external forcings was investigated by replacing or combining them with a fixed number of BSplines in the latent equation. Two different validation exercises confirm that it is feasible to improve the predictive ability of traditional external forcing models.





Browse Publish About

(日)

RESEARCH ARTICLE

Chagas disease mortality in Brazil: A Bayesian analysis of ageperiod-cohort effects and forecasts for two decades

Taynāna César Simões 🔤 🔄, Laiane Félix Borges, Auzenda Conceição Parreira de Assis, Maria Vitórias Silva, Juliano dos Santos, Karina Cardoso Meira 🚥

Version 2

Published: September 28, 2018 • https://doi.org/10.1371/journal.pntd.0006798









Experiences in Transplanting Wood Ants into Plantations for Integrated Pest Management

Jesper Stern Nielsen, Mogens Gissel Nielsen, Joachim Offenberg

Abstract

Ants can function efficiently as biocontrol agents in open field horticulture. Temperate wood ants can control forest pests, including species damaging forest regeneration plots and fruit plantations. Thus, they possess potential as biocontrol agents in open field horticulture, if they can persist in these systems. Here we present observationson activity and survival of wood ants transplanted from forests into different types of plantations. Mound fragments were transplanted into a confire seedling plot, an organic and a conventional Christmas tree plantation, and

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 6 / 135



Malaria Journal



Methodology Open Access

malariaAtlas: an R interface to global malariometric data hosted by the Malaria Atlas Project

Daniel A. Pfeffer, Timothy C. D. Lucas ≌, Daniel May, Joseph Harris, Jennifer Rozier, Katherine A. Twohig, Ursula Dalrymple, Carlos A. Guerra, Catherine L. Moyes, Mike Thorn, Michele Nguyen, Samir Bhatt, Ewan Cameron, Daniel J. Weiss, Rosalind E. Howes, Katherine E. Battle, Harry S. Gibson and Peter W. Gething

Malaria Journal 2018 17:352

https://doi.org/10.1186/s12936-018-2500-5 © The Author(s) 2018

Received: 3 July 2018 Accepted: 29 September 2018 Published: 5 October 2018

A B F A B F





Access by King Abdullah University of Science and Technology

JOURNALS $\, \smallsetminus \,$

Journal of Ecology



Research Article 🔂 Full Access

Larger plants promote a greater diversity of symbiotic nitrogen-fixing soil bacteria associated with an Australian

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 6 / 135



A three-stage model for short-term extreme wind speed probabilistic forecasting

Daniela Castro-Camilo¹, Raphaël Huser¹, and Håvard Rue¹

October 8, 2018

Abstract

Renewable sources of energy such as wind power have become a sustainable alternative to fossil fuel-based energy. However, the uncertainty and fluctuation of the wind speed derived from its intermittent nature bring a great threat to the wind power production stability, and to the

イロト イポト イヨト イヨト 一日



nature > scientific reports > articles > article

SCIENTIFIC REPORTS

Article | OPEN | Published: 11 October 2018

Spatiotemporal dynamics and risk factors for human Leptospirosis in Brazil

Oswaldo Santos Baquero 🖾 & Gustavo Machado 🖾

Scientific Reports 8, Article number: 15170 (2018) Download Citation 🕹

.





RESEARCH ARTICLE 🔂 Full Access

A spatio-temporal approach to estimate patterns of climate change

M. P. Laurini 🔀

First published: 11 October 2018 | https://doi.org/10.1002/env.2542

< □ > < 同

- E - - E -



PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B

search		
--------	--	--

Advanc

BIOLOGICAL SCIENCES

Home Content Information for About us Sign up Propose an iss	ie
--	----



Interactive effects of tree size, crown exposure and logging on drought-induced mortality

Alexander Shenkin, Benjamin Bolker, Marielos Peña-Claros, Juan Carlos Licona, Nataly Ascarrunz, Francis E. Putz

Published 8 October 2018. DOI: 10.1098/rstb.2018.0189





Coláiste na Tríonóide, Baile Átha Cliath Trinity College Dublin Ollscoil Átha Cliath | The University of Dublin

The Environmental Epidemiology of

Amyotrophic Lateral Sclerosis in Europe

A dissertation submitted to Trinity College Dublin in fulfilment for the award of

Doctor of Philosophy (PhD)

James PK Rooney

B.Sc. , M.B. B.Ch. B.A.O. , M.Sc.

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 6 / 135

Activities



Public discussion group

R-i 30 or	nla disc f 1382 top	ussion group Shared publicly ics (99+ unread)	Membership and email settings	Members · About 💿
	-	CAR as a linear combination (11) By Román Aguirre-Pérez - 11 posts	- 18 views	Oct 19
	•	Problem of the Value of hyperparameter in Tokyo Rainfall Case (2) By yuki - 2 posts - 8 views		
		Precision (6) By endale alemayehu - 6 posts - 29	views	Oct 15
	•	inlabru besag spatial model synta By TDM - 8 posts - 20 views	их (8)	Oct 15
	•	exact log Marginal likelihood (2) By s.p.usa22@gmail.com - 2 posts	- 4 views	Oct 14
	•	BYM Model & Space - time interact By omdess2016@gmail.com - 2 pos	sts - 14 views	Oct 12
	:	How to deal with area fractions in By Øyvind - 5 posts - 9 views	spatial analysis? (5)	Oct 12
	•	Multinomial data analyses with di	fferent category effect (2)	

E ● E の Q C Oct 2018 7 / 135

臣▶ ★ 臣▶

Activities



Public discussion group

R-inla disc 30 of 1382 topi	USSION GROUP Shared publicly Membership and email settings cs (99+ unread)	Members · About 💿
	CAR as a linear combination (11) By Román Aguirre-Pérez - 11 posts - 18 views	Oct 19
	Problem of the Value of hyperparameter in Tokyo Rainfall Case By yuki - 2 posts - 8 views	(2) Oct 15
	Precision (6) By endale alemayehu - 6 posts - 29 views	Oct 15
	inlabru besag spatial model syntax (8) By TDM - 8 posts - 20 views	Oct 15
	exact log Marginal likelihood (2) By s.p.usa22@gmail.com - 2 posts - 4 views	Oct 14
	BYM Model & Space - time interactions (2) By omdess2016@gmail.com - 2 posts - 14 views	Oct 12
	How to deal with area fractions in spatial analysis? (5) By Øyvind - 5 posts - 9 views	Oct 12
	Multinomial data analyses with different category effect (2)	

Visits to www.r-inla.org

How are your active users trending over time?



Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 7 / 135

-

Locations of users



Presence



Oct 2018 8 / 135

3 🕨 🖌 3

Locations of users



Countries



С	ountry 🕐	Users ?	\downarrow
		25 % of Total: 100.00%	5,039 (25,039)
1.	United States	6,474	(25.62%)
2.	🔡 United Kingdom	2,945	(11.66%)
3.	🛃 Canada	1,427	(5.65%)
4.	S Brazil	1,205	(4.77%)
5.	드 Spain	993	(3.93%)
6.	📰 Australia	872	(3.45%)
7.	France	855	(3.38%)
8.	📕 Germany	791	(3.13%)
9.	Norway	718	(2.84%)
10.	China China	706	(2.79%)

Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 8 / 135

The code



Respository



◆ロト ◆聞ト ◆臣ト ◆臣ト

The code



Respository

> н	нC	🟠 🧰 Atlassian, Inc. (US)	bitbucket.org/hrue/r-inla/src/default/
v		R-INLA	Håvard Rue R-INLA
	\circ	Source	This is the respoitory for the R-INLA package and related projects
	¢	Commits	
	ţ	Branches	🕼 default 🗸 Filter files
	រែ	Pull requests	I
	¢	Pipelines	Name Size Last commit
	P	Deployments	build-configs
	₽	Issues	build-user/linux
	F	Wiki	extlibs
	Ð	Downloads	fmesher
		Boards	gmrflib
	0	Settings	inla-remote

Commits

Commits

₽ All	branches +			0	Q, Find	commits
	Author	Commit	Message			Date
	🍘 Håvard Rue	257bb3a	Added tag Version_18.10.17 for changeset c386e011c5bd			5 days ago
	Håvard Rue	c385e01	Updated NEWS	Jpdated NEWS Straton_10		5 days ago
	🌘 Hávard Rue	3ed192a	Removed tag Version_18.10.17			5 days ago
	Hávard Rue	5d44d47	Added tag Version_18.10.17 for changeset 8679312c23b1			5 days ago
	Håvard Rue	8679312	Removed tag Version_18.10.17			5 days ago
ļ	🍘 Håvard Rue	6496454 M	Merge from small-fixes			5 days ago
	🍘 Håvard Rue	a684ea1	Small fix to my.update() due to the new export of cl.	þ small	-fixes	5 days ago
	🍈 Håvard Rue	d98ddbb M	Merge from default	D small		5 days ago
(Hávard Rue 3bbdfd8		Added tag Version_18.10.17 for changeset 7c7a78ea318a		5 days ago	
t	Håvard Rue	2cf532b M	Merge from default	1	f 02v2	5 days ago
1	🍘 Håvard Rue	7c7a78e	Ran indent			5 days ago
	🍘 Håvard Rue	236666f M	Merge from dmatern			5 days ago
A) -	🍘 Håvard Rue	1795319	Cleaned up some of the new code	D di	satern	5 days ago
1	Håvard Rue	b7a2e3c M	Merge from default	D de		5 days ago
	🍘 Hávard Rue	384d32d	Forgot a debug statement			2018-10-16
	Håvard Rue	63e4fe2	Ran top make. Export the inla-class as suggested by	T.Onkelinx, th	han	2018-10-16

< □ ▶ < 四

▶ 《 臣 ▶ 《 臣 ▶











Håvard Rue (haavard.rue@kaust.edu.sa)





Håvard Rue (haavard.rue@kaust.edu.sa)







Håvard Rue (haavard.rue@kaust.edu.sa)





























Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa











Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa











Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa


Some of the people, directly and indirectly involved



Oct 2018 10 / 135

Part I

Background and Introduction

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 11 / 135



- The issue of Bayesian computing is not "solved" even though MCMC is available
- Hierarcical models are more difficult for MCMC
- A main obstacle for Bayesian modelling is the issue of "Bayesian computing"
- There are (somewhat) generic tools are available JAGS/stan, based on MCMC
- Still slower than we would like them to be



• The issue of Bayesian computing is not "solved" even though MCMC is available

• Hierarcical models are more difficult for MCMC

- A main obstacle for Bayesian modelling is the issue of "Bayesian computing"
- There are (somewhat) generic tools are available JAGS/stan, based on MCMC
- Still slower than we would like them to be



- The issue of Bayesian computing is not "solved" even though MCMC is available
- Hierarcical models are more difficult for MCMC
- A main obstacle for Bayesian modelling is the issue of "Bayesian computing"
- There are (somewhat) generic tools are available JAGS/stan, based on MCMC
- Still slower than we would like them to be



- The issue of Bayesian computing is not "solved" even though MCMC is available
- Hierarcical models are more difficult for MCMC
- A main obstacle for Bayesian modelling is the issue of "Bayesian computing"
- There are (somewhat) generic tools are available JAGS/stan, based on MCMC
- Still slower than we would like them to be



- The issue of Bayesian computing is not "solved" even though MCMC is available
- Hierarcical models are more difficult for MCMC
- A main obstacle for Bayesian modelling is the issue of "Bayesian computing"
- There are (somewhat) generic tools are available JAGS/stan, based on MCMC
- Still slower than we would like them to be



GLM/GAM/GLMM/GAMM/++

• Perhaps the most important class of statistical models

- Many "models" can be cast in to this class without knowing
- No good (enough) MCMC solution around
- Many suggested approaches does not scale well computationally



GLM/GAM/GLMM/GAMM/++

- Perhaps the most important class of statistical models
- Many "models" can be cast in to this class without knowing
- No good (enough) MCMC solution around
- Many suggested approaches does not scale well computationally



GLM/GAM/GLMM/GAMM/++

- Perhaps the most important class of statistical models
- Many "models" can be cast in to this class without knowing
- No good (enough) MCMC solution around
- Many suggested approaches does not scale well computationally



GLM/GAM/GLMM/GAMM/++

- Perhaps the most important class of statistical models
- Many "models" can be cast in to this class without knowing
- No good (enough) MCMC solution around
- Many suggested approaches does not scale well computationally

Bayesian GLM/GAM/GLMM/GAMM/+++



Linear predictor

$$oldsymbol{\eta} = \mu \mathbf{1} + oldsymbol{A}oldsymbol{eta} + \sum_i oldsymbol{B}_i oldsymbol{v}_i + oldsymbol{\epsilon}$$

where

- **A**: covariates, with fixed effects $\boldsymbol{\beta} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma})$
- **B**_i: weights, with random effects $\mathbf{v}_i \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$
- ϵ_i : possible Gaussian noise

Observations

$$\mathbf{y} \sim \pi(\mathbf{y} \mid \boldsymbol{\eta},) = \prod_{i} \pi(y_i \mid \eta_i)$$

▶ ∢ ⊒

Bayesian GLM/GAM/GLMM/GAMM/+++



Linear predictor

$$oldsymbol{\eta} = \mu \mathbf{1} + oldsymbol{A}oldsymbol{eta} + \sum_i oldsymbol{B}_i oldsymbol{v}_i + oldsymbol{\epsilon}$$

where

- **A**: covariates, with fixed effects $\boldsymbol{\beta} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma})$
- **B**_i: weights, with random effects $\mathbf{v}_i \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$
- ϵ_i : possible Gaussian noise

Observations

$$\mathbf{y} \sim \pi(\mathbf{y} \mid \boldsymbol{\eta},) = \prod_{i} \pi(y_i \mid \eta_i)$$

3 🕨 🖌 3

Example I



Smoothing of binary/integer time-series



$$p_t = \frac{\exp(\eta_t)}{1 + \exp(\eta_t)}$$

э

• □ > • □ > • □ > •



Smoothing of binary/integer time-series



• Data is sequence of 0, 1 and 2's

• Binomial data where probability for a success *p*_t, depends on time *t*

$$p_t = \frac{\exp(\eta_t)}{1 + \exp(\eta_t)}$$

• Linear predictor $\eta_t = \mu + \beta c_t + u_t + v_t$, $t = 1, \dots, n_t$

Example I



Smoothing of binary/integer time-series



- Data is sequence of 0, 1 and 2's
- Binomial data where probability for a success p_t , depends on time t ۲

$$p_t = \frac{\exp(\eta_t)}{1 + \exp(\eta_t)}$$

• Linear predictor $\eta_t = \mu + \beta c_t + u_t + v_t, \quad t = 1, \dots, n$



Smoothing of binary/integer time-series



- Data is sequence of 0, 1 and 2's
- Binomial data where probability for a success *p*_t, depends on time *t*

$$p_t = \frac{\exp(\eta_t)}{1 + \exp(\eta_t)}$$

• Linear predictor $\eta_t = \mu + \beta c_t + u_t + v_t$, $t = 1, \dots, n$



We can reinterpret the model as

$$\begin{array}{rcl} \boldsymbol{\theta} & \sim & \pi(\boldsymbol{\theta}) \\ \boldsymbol{x} \mid \boldsymbol{\theta} & \sim & \pi(\boldsymbol{x} \mid \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma}(\boldsymbol{\theta})) \\ \boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{\theta} & \sim & \prod_{i} \pi(y_{i} \mid \eta_{i}, \boldsymbol{\theta}) \end{array}$$

dim(x) could be large 10²-10⁵
 dim(θ) is small 1-5

F 4 3 F 4 3 F

< A



We can reinterpret the model as

$$\begin{array}{rcl} \boldsymbol{\theta} & \sim & \pi(\boldsymbol{\theta}) \\ \boldsymbol{x} \mid \boldsymbol{\theta} & \sim & \pi(\boldsymbol{x} \mid \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma}(\boldsymbol{\theta})) \\ \boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{\theta} & \sim & \prod_{i} \pi(y_{i} \mid \eta_{i}, \boldsymbol{\theta}) \end{array}$$

- dim(\boldsymbol{x}) could be large 10²-10⁵
- dim(θ) is small 1-5

3 1 4 3

Precision matrix (η , \boldsymbol{u} , \boldsymbol{v} , μ , β) N = 100, M = 5.



Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 17 / 135

御下 イヨト イヨ

Reordered precision matrix



Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 17 / 135 Cholesky triangle of the reordered precision matrix



Oct 2018 17 / 135

Example II: Disease mapping

- Data y_i ~ Poisson(E_iexp(η_i))
 Log-relative risk
 - $\eta_i = \mu + u_i + v_i + f(c_i)$
- Structured/Spatial component **u**
- Unstructured component v
- Smooth effect of a covariate *c*





.



Example II: Disease mapping

- Data $y_i \sim \text{Poisson}(E_i exp(\eta_i))$
- Log-relative risk $\eta_i = \mu + u_i + v_i + f(c_i)$
- Structured/Spatial component **u**
- Unstructured component v
- Smooth effect of a covariate *c*





Example II: Disease mapping

- Data $y_i \sim \text{Poisson}(E_i exp(\eta_i))$
- Log-relative risk

 $\eta_i = \mu + u_i + v_i + f(c_i)$

- Structured/Spatial component **u**
- Unstructured component v
- Smooth effect of a covariate *c*





Example II: Disease mapping

- Data $y_i \sim \text{Poisson}(E_i exp(\eta_i))$
- Log-relative risk
 - $\eta_i = \mu + u_i + v_i + f(c_i)$
- Structured/Spatial component u
- Unstructured component v
- Smooth effect of a covariate *c*





Example II: Disease mapping

- Data $y_i \sim \text{Poisson}(E_i exp(\eta_i))$
- Log-relative risk

 $\eta_i = \mu + u_i + v_i + f(c_i)$

- Structured/Spatial component **u**
- Unstructured component v
- Smooth effect of a covariate *c*





Precision matrix $(\boldsymbol{\eta}, \boldsymbol{u}, \boldsymbol{v}, \mu, \boldsymbol{f})$



Oct 2018 19 / 135

A (1) > A (2) > A

Reordered precision matrix



Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 19 / 135

Cholesky triangle of the reordered precision matrix



Oct 2018 19 / 135



We can reinterpret the model as

$$\begin{array}{rcl} \boldsymbol{\theta} & \sim & \pi(\boldsymbol{\theta}) \\ \boldsymbol{x} \mid \boldsymbol{\theta} & \sim & \pi(\boldsymbol{x} \mid \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma}(\boldsymbol{\theta})) \\ \boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{\theta} & \sim & \prod_{i} \pi(y_{i} \mid \eta_{i}, \boldsymbol{\theta}) \end{array}$$

- dim(\boldsymbol{x}) could be large 10²-10⁵
- dim(θ) is small 1-5

글 🖌 🖌 글 🗄

What we have learned so far (I)



This model-construct

$$\begin{array}{rcl} \boldsymbol{\theta} & \sim & \pi(\boldsymbol{\theta}) \\ \boldsymbol{x} \mid \boldsymbol{\theta} & \sim & \pi(\boldsymbol{x} \mid \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma}(\boldsymbol{\theta})) \\ \boldsymbol{y} \mid \boldsymbol{x}, \boldsymbol{\theta} & \sim & \prod_{i} \pi(y_{i} \mid \eta_{i}, \boldsymbol{\theta}) \end{array}$$

occurs in seemingly unrelated, statistical models.

Latent Gaussian models!

Dynamic linear models

- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models







Dynamic linear models

Stochastic volatility

- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models

- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models





- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models




- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models





- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models



- Dynamic linear models
- Stochastic volatility
- Generalised linear (mixed) models
- Generalised additive (mixed) models
- Measurement error models
- Spline smoothing
- Semiparametric regression
- Space-varying (semiparametric) regression models
- Disease mapping
- Log-Gaussian Cox-processes
- Model-based geostatistics (*)
- Spatio-temporal models
- Survival analysis
- Joint survival/longitudional models
- +++



What we have learned so far (II)

The precision matrix of the latent field

$$oldsymbol{Q}(oldsymbol{ heta}) = oldsymbol{\Sigma}(oldsymbol{ heta})^{-1}$$

is sparse and this will play a key role!

Two important benefits

- Building models through conditioning ("hierarchical models")
- Computational



What we have learned so far (II)

The precision matrix of the latent field

$$\boldsymbol{Q}(\boldsymbol{ heta}) = \boldsymbol{\Sigma}(\boldsymbol{ heta})^{-1}$$

is sparse and this will play a key role!

Two important benefits

- Building models through conditioning ("hierarchical models")
- Computational



Building models through conditioning



•
$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_x^{-1})$$

• $\boldsymbol{y} | \boldsymbol{x} \sim \mathcal{N}(\boldsymbol{x}, \boldsymbol{Q}_y^{-1})$

then

$$\mathbf{Q}_{(x,y)} = \begin{bmatrix} \mathbf{Q}_x + \mathbf{Q}_y & -\mathbf{Q}_y \\ -\mathbf{Q}_y & \mathbf{Q}_y \end{bmatrix}$$

Not so nice expressions using the Covariance-matrix

Building models through conditioning



lf

•
$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_x^{-1})$$

• $\boldsymbol{y} | \boldsymbol{x} \sim \mathcal{N}(\boldsymbol{x}, \boldsymbol{Q}_y^{-1})$

then

$$\mathbf{Q}_{(\mathbf{x},\mathbf{y})} = \begin{bmatrix} \mathbf{Q}_{x} + \mathbf{Q}_{y} & -\mathbf{Q}_{y} \\ -\mathbf{Q}_{y} & \mathbf{Q}_{y} \end{bmatrix}$$

Not so nice expressions using the Covariance-matrix

Building models through conditioning



lf

•
$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}_x^{-1})$$

• $\boldsymbol{y} | \boldsymbol{x} \sim \mathcal{N}(\boldsymbol{x}, \boldsymbol{Q}_y^{-1})$

then

$$\mathbf{Q}_{(\mathbf{x},\mathbf{y})} = \begin{bmatrix} \mathbf{Q}_x + \mathbf{Q}_y & -\mathbf{Q}_y \\ -\mathbf{Q}_y & \mathbf{Q}_y \end{bmatrix}$$

Not so nice expressions using the Covariance-matrix



• Models we have seen gives a sparse precision matrix

- These are much faster to compute with, than dense matrices
- Special case: Kalman-filter algorithms

Tasks:

- Factorize **Q** into $\mathbf{Q} = \mathbf{L}\mathbf{L}^T$ (Cholesky)
- Solve Qx = b, Lx = b or $L^T x = b$
- Compute diag(Q⁻¹)



- Models we have seen gives a sparse precision matrix
- These are much faster to compute with, than dense matrices
- Special case: Kalman-filter algorithms

- Factorize **Q** into $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$ (Cholesky)
- Solve Qx = b, Lx = b or $L^T x = b$
- Compute diag(Q⁻¹)



- Models we have seen gives a sparse precision matrix
- These are much faster to compute with, than dense matrices
- Special case: Kalman-filter algorithms

- Factorize **Q** into $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$ (Cholesky)
- Solve Qx = b, Lx = b or $L^T x = b$
- Compute diag(Q⁻¹)



- Models we have seen gives a sparse precision matrix
- These are much faster to compute with, than dense matrices
- Special case: Kalman-filter algorithms

- Factorize **Q** into $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$ (Cholesky)
- Solve Qx = b, Lx = b or $L^T x = b$
- Compute diag(Q⁻¹)



- Models we have seen gives a sparse precision matrix
- These are much faster to compute with, than dense matrices
- Special case: Kalman-filter algorithms

- Factorize **Q** into $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$ (Cholesky)
- Solve Qx = b, Lx = b or $L^T x = b$
- Compute diag(**Q**⁻¹)



- Models we have seen gives a sparse precision matrix
- These are much faster to compute with, than dense matrices
- Special case: Kalman-filter algorithms

Tasks:

- Factorize **Q** into $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$ (Cholesky)
- Solve Qx = b, Lx = b or $L^T x = b$

• Compute diag(**Q**⁻¹)



- Models we have seen gives a sparse precision matrix
- These are much faster to compute with, than dense matrices
- Special case: Kalman-filter algorithms

- Factorize **Q** into $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$ (Cholesky)
- Solve Qx = b, Lx = b or $L^T x = b$
- Compute diag(Q⁻¹)



Cholesky factorization of "sparse" SPD¹ matrix

• Time: $\mathcal{O}(n)$

properties

- Space: $\mathcal{O}(n^{3/2})$
- Space-time: $\mathcal{O}(n^2)$

¹Symmetric and positive definite

Håvard Rue (haavard.rue@kaust.edu.sa)

bavescomp.kaust.edu.sa





Numerical algorithms for sparse matrices: scaling properties

Cholesky factorization of "sparse" SPD¹ matrix

- Time: $\mathcal{O}(n)$
- Space: $\mathcal{O}(n^{3/2})$
- Space-time: $\mathcal{O}(n^2)$

¹Symmetric and positive definite

Håvard Rue (haavard.rue@kaust.edu.sa)

bavescomp.kaust.edu.sa



Numerical algorithms for sparse matrices: scaling properties

Cholesky factorization of "sparse" SPD¹ matrix

- Time: O(n)
- Space: *O*(*n*^{3/2})
- Space-time: $\mathcal{O}(n^2)$

This is to be compared with general $\mathcal{O}(n^3)$ algorithm for the Cholesky factorization of a SPD dense matrix.

¹Symmetric and positive definite

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa



Numerical algorithms for sparse matrices: scaling properties

Cholesky factorization of "sparse" SPD¹ matrix

- Time: O(n)
- Space: *O*(*n*^{3/2})
- Space-time: $\mathcal{O}(n^2)$

This is to be compared with general $\mathcal{O}(n^3)$ algorithm for the Cholesky factorization of a SPD dense matrix.

¹Symmetric and positive definite

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa



Numerical algorithms for sparse matrices: scaling properties

Cholesky factorization of "sparse" SPD¹ matrix

- Time: O(n)
- Space: *O*(*n*^{3/2})
- Space-time: $\mathcal{O}(n^2)$

This is to be compared with general $\mathcal{O}(n^3)$ algorithm for the Cholesky factorization of a SPD dense matrix.

¹Symmetric and positive definite

Gaussian Markov random fields



• Gaussians with a sparse precision matrix are called *Gaussian Markov* random fields (GMRFs)

- Good computational properties through numerical algorithms for sparse matrices
- Very useful in other settings as well

Gaussian Markov random fields



- Gaussians with a sparse precision matrix are called *Gaussian Markov* random fields (GMRFs)
- Good computational properties through numerical algorithms for sparse matrices
- Very useful in other settings as well

Gaussian Markov random fields



- Gaussians with a sparse precision matrix are called *Gaussian Markov* random fields (GMRFs)
- Good computational properties through numerical algorithms for sparse matrices
- Very useful in other settings as well



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++

イロト イヨト イヨト



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++

(日)



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++

イロト イヨト イヨト



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++

イロト イヨト イヨト



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++
Summary



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++

Summary



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++

Summary



Three main ingredients in INLA

- Gaussian Markov random fields
- Latent Gaussian models
- Laplace approximations

which together (and ++++...) gives a very very nice tool for Bayesian inference

- quick
- accurate (relative error)
- good scaling properties
- +++

Spatial survival: example



Leukaemia survival data (Henderson et al, 2002, JASA), 1043 cases.



Fig 1. Leukaemia survival data: districts of Northwest England and locations of the observations.

Spatial survival: example



log(hazard) = log(baseline)
+f(white blood cell count)
+f(deprivation index)
+f(spatial)
+sex

+sex

+age



Oct 2018 30 / 135

R-code



data(Leuk)
g = system.file("demodata/Leuk.graph", package="INLA")
formula = inla.surv(Leuk\$time, Leuk\$cens) ~ sex + age +
 f(inla.group(wbc), model="rw2") +
 f(inla.group(tpi), model="rw2") +
 f(district, model="besag", graph = g) +

r = inla(formula, family="coxph", data = Leuk)

plot(r)

▲ □ ▶ ▲ □ ▶ ▲ □ ▶ ● ● ● ● ● ● ●



■ ▶ ■ つへの Oct 2018 32/135

inla.group(wbc)



PostMean 0.025% 0.5% 0.975%

(Ξ) Ξ
 <l

inla.group(tpi)



PostMean 0.025% 0.5% 0.975%

bayescomp.kaust.edu.sa



Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 32 / 135

590

◆ロ > ◆舂 > ◆臣 > ◆臣 > ─ 臣



baseline.hazard

PostMean 0.025% 0.5% 0.975%

Some internal statistics



Running time on my laptop: 2.3 seconds

- Factorise **Q** (dim = 2453): 455 times
- Solve *Qx* = *b*: 3160 times
- Partially invert **Q**: 28 times

Part II

Theory and methods

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 34 / 135

医子宫医子宫

What is a Gaussian Markov random field (GMRF)?



A GMRF is a simple construct

• A normal distributed random vector

$$\boldsymbol{x} = (x_1, \ldots, x_n)^T$$

• Additional Markov properties:

$$x_i \perp x_j \mid \mathbf{x}_{-ij}$$

x_i and *x_j* are conditional independent (CI).

Oct 2018 35 / 135

What is a Gaussian Markov random field (GMRF)?



A GMRF is a simple construct

• A normal distributed random vector

$$\boldsymbol{x} = (x_1, \ldots, x_n)^T$$

• Additional Markov properties:

$$x_i \perp x_j \mid \mathbf{x}_{-ij}$$

 x_i and x_j are conditional independent (CI).

Oct 2018 35 / 135

If $x_i \perp x_j \mid \mathbf{x}_{-ij}$ for a set of $\{i, j\}$, then we need to constrain the parametrisation of the GMRF.

- Covariance matrix: difficult
- Precision matrix: easy

3 1 4 3

If $x_i \perp x_j \mid \mathbf{x}_{-ij}$ for a set of $\{i, j\}$, then we need to constrain the parametrisation of the GMRF.

- Covariance matrix: difficult
- Precision matrix: easy

3 1 4 3



Conditional independence and the precision matrix

The density of a zero mean Gaussian

$$\pi(\mathbf{x}) \propto |\mathbf{Q}|^{1/2} \exp\left(-\frac{1}{2}\mathbf{x}^{\mathsf{T}}\mathbf{Q}\mathbf{x}\right)$$

Constraining the parametrisation to obey CI properties

Theorem

$$x_i \perp x_j \mid \boldsymbol{x}_{-ij} \quad \Longleftrightarrow \quad Q_{ij} = 0$$

Oct 2018 37 / 135



Conditional independence and the precision matrix

The density of a zero mean Gaussian

$$\pi(\mathbf{x}) \propto |\mathbf{Q}|^{1/2} \exp\left(-\frac{1}{2}\mathbf{x}^{T}\mathbf{Q}\mathbf{x}\right)$$

Constraining the parametrisation to obey CI properties

Theorem

$$x_i \perp x_j \mid \boldsymbol{x}_{-ij} \quad \Longleftrightarrow \quad Q_{ij} = 0$$

Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 37 / 135

Global Markov property



Let **x** be a GMRF wrt $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. The global Markov property:

$$\mathbf{x}_A \perp \mathbf{x}_B \mid \mathbf{x}_C$$

for all disjoint sets *A*, *B* and *C* where *C* separates *A* and *B*, and *A* and *B* are non-empty.



Oct 2018 38 / 135

Simple example of a GMRF

Auto-regressive process of order 1

$$x_t | x_{t-1}, \ldots, x_1 \sim \mathcal{N}(\phi x_{t-1}, 1), \quad t = 2, \ldots, n$$

and $x_1 \sim \mathcal{N}(0, (1 - \phi^2)^{-1}).$



Tridiagonal precision matrix

$$\mathbf{Q} = \begin{pmatrix} 1 & -\phi \\ -\phi & 1+\phi^2 & -\phi \\ & \ddots & \ddots & \ddots \\ & -\phi & 1+\phi^2 & -\phi \\ & & -\phi & 1 \end{pmatrix}$$



Simple example of a GMRF

Auto-regressive process of order 1

$$x_t | x_{t-1}, \ldots, x_1 \sim \mathcal{N}(\phi x_{t-1}, 1), \quad t = 2, \ldots, n$$

and $x_1 \sim \mathcal{N}(0, (1 - \phi^2)^{-1}).$



Tridiagonal precision matrix

$$\mathbf{Q} = \begin{pmatrix} 1 & -\phi \\ -\phi & 1 + \phi^2 & -\phi \\ & \ddots & \ddots & \ddots \\ & -\phi & 1 + \phi^2 & -\phi \\ & & -\phi & 1 \end{pmatrix}$$



Part III

Simulation algorithms for GMRFs. Numerical methods for sparse matrices.

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 40 / 135

Cholesky factorisation



 If *A* > 0 be a *n* × *n* positive definite matrix, then there exists a unique Cholesky triangle *L*, such that *L* is a lower triangular matrix, and

$$\mathbf{A} = \mathbf{L}\mathbf{L}^{\mathsf{T}}$$

- Computing L costs n³/3 flops.
- This factorisation is the basis for solving systems like

for k right hand sides, or equivalently, computing

$$x = A^{-1}b$$
 or $X = A^{-1}B$

Cholesky factorisation



 If *A* > 0 be a *n* × *n* positive definite matrix, then there exists a unique Cholesky triangle *L*, such that *L* is a lower triangular matrix, and

$$\mathbf{A} = \mathbf{L}\mathbf{L}^{\mathsf{T}}$$

- Computing **L** costs $n^3/3$ flops.
- This factorisation is the basis for solving systems like

Ax = b or AX = B

for k right hand sides, or equivalently, computing

$$x = A^{-1}b$$
 or $X = A^{-1}B$

Cholesky factorisation



 If *A* > 0 be a *n* × *n* positive definite matrix, then there exists a unique Cholesky triangle *L*, such that *L* is a lower triangular matrix, and

$$\mathbf{A} = \mathbf{L}\mathbf{L}^{T}$$

- Computing **L** costs $n^3/3$ flops.
- This factorisation is the basis for *solving* systems like

for k right hand sides, or equivalently, computing

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$$
 or $\boldsymbol{X} = \boldsymbol{A}^{-1}\boldsymbol{B}$

Algorithm 1 Solving Ax = b where A > 0

- 1: Compute the Cholesky factorisation, $\mathbf{A} = \mathbf{L}\mathbf{L}^{T}$
- 2: Solve *Lv* = *b*
- 3: Solve $\boldsymbol{L}^T \boldsymbol{x} = \boldsymbol{v}$
- 4: Return x

A B F A B F

Algorithm 1 Solving Ax = b where A > 0

- 1: Compute the Cholesky factorisation, $\mathbf{A} = \mathbf{L}\mathbf{L}^{T}$
- 2: Solve *Lv* = *b*
- 3: Solve $\boldsymbol{L}^T \boldsymbol{x} = \boldsymbol{v}$
- 4: Return x

Step 2 is called *forward-substitution* and cost $O(n^2)$ flops.



The solution **v** is computed in a forward-loop

$$v_i = \frac{1}{L_{ii}}(b_i - \sum_{j=1}^{i-1} L_{ij}v_j), \quad i = 1, \dots, n$$
 (1)

Algorithm 1 Solving Ax = b where A > 0

- 1: Compute the Cholesky factorisation, $\mathbf{A} = \mathbf{L}\mathbf{L}^{T}$
- 2: Solve **Lv** = **b**
- 3: Solve $\boldsymbol{L}^T \boldsymbol{x} = \boldsymbol{v}$
- 4: Return x

Step 3 is called *back-substitution* and costs $O(n^2)$ flops.



The solution **x** is computed in a backward-loop

$$x_i = \frac{1}{L_{ii}}(v_i - \sum_{j=i+1}^n L_{ji}x_j), \quad i = n, \dots, 1$$
 (2)

To compute $A^{-1}B$ where **B** is a $n \times k$ matrix, we do this by computing the solution **X** of

$$AX_j = B_j$$

for each of the *k* columns of *X*.

Algorithm 2 Solving *AX* = *B* where *A* > 0

1: Compute the Cholesky factorisation, $\mathbf{A} = \mathbf{L}\mathbf{L}^{T}$

2: **for** *j* = 1 to *k* **do**

4: Solve
$$\boldsymbol{L}^T \boldsymbol{X}_i = \boldsymbol{V}$$

- 5: end for
- 6: Return X

• • = • • = •

To compute $\mathbf{A}^{-1}\mathbf{B}$ where \mathbf{B} is a $n \times k$ matrix, we do this by computing the solution \mathbf{X} of

$$AX_j = B_j$$

for each of the *k* columns of *X*.

Algorithm 2 Solving AX = B where A > 0

- 1: Compute the Cholesky factorisation, $\mathbf{A} = \mathbf{L}\mathbf{L}^{T}$
- 2: **for** *j* = 1 to *k* **do**
- 3: Solve $Lv = B_j$
- 4: Solve $\boldsymbol{L}^T \boldsymbol{X}_j = \boldsymbol{v}$
- 5: **end for**
- 6: Return X

3 1 4 3

Sample $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{Q}^{-1})$

If
$$\boldsymbol{Q} = \boldsymbol{L} \boldsymbol{L}^T$$
 and $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$, then \boldsymbol{x} defined by

$$\boldsymbol{L}^T \boldsymbol{x} = \boldsymbol{z}$$

has covariance

$$\operatorname{Cov}(\boldsymbol{x}) = \operatorname{Cov}(\boldsymbol{L}^{-T}\boldsymbol{z}) = (\boldsymbol{L}\boldsymbol{L}^{T})^{-1} = \boldsymbol{Q}^{-1}$$

Algorithm 3 Sampling $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{Q}^{-1})$

- 1: Compute the Cholesky factorisation, $Q = LL^T$
- 2: Sample **z** ∼ *N*(**0**, *I*)
- 3: Solve $\boldsymbol{L}^T \boldsymbol{v} = \boldsymbol{z}$
- 4: Compute $\mathbf{x} = \mathbf{\mu} + \mathbf{v}$
- 5: Return x



ト くきト くきト



Sample $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{Q}^{-1})$

If
$$\boldsymbol{Q} = \boldsymbol{L} \boldsymbol{L}^T$$
 and $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$, then \boldsymbol{x} defined by

$$\boldsymbol{L}^T \boldsymbol{x} = \boldsymbol{z}$$

has covariance

$$\operatorname{Cov}(\boldsymbol{x}) = \operatorname{Cov}(\boldsymbol{L}^{-T}\boldsymbol{z}) = (\boldsymbol{L}\boldsymbol{L}^{T})^{-1} = \boldsymbol{Q}^{-1}$$

Algorithm 3 Sampling $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{Q}^{-1})$

- 1: Compute the Cholesky factorisation, $\boldsymbol{Q} = \boldsymbol{L} \boldsymbol{L}^{T}$
- 2: Sample $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$
- 3: Solve $\mathbf{L}^T \mathbf{v} = \mathbf{z}$
- 4: Compute $\mathbf{x} = \boldsymbol{\mu} + \boldsymbol{v}$
- Return x 5٠



ヨトィヨト



The log-density is

$$\log \pi(\boldsymbol{x}) = -\frac{n}{2}\log 2\pi + \sum_{i=1}^{n}\log L_{ii} - \frac{1}{2}(\underbrace{\boldsymbol{x} - \boldsymbol{\mu}})^{T} \boldsymbol{Q}(\boldsymbol{x} - \boldsymbol{\mu})}_{=q}$$

If **x** is sampled, then

$$q = \mathbf{z}^T \mathbf{z}$$

otherwise, compute this term as

•
$$\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{\mu}$$

•
$$q = \mathbf{u}^T \mathbf{v}$$

The log-density is

$$\log \pi(\boldsymbol{x}) = -\frac{n}{2}\log 2\pi + \sum_{i=1}^{n}\log L_{ii} - \frac{1}{2}(\underbrace{\boldsymbol{x}-\boldsymbol{\mu}})^{T}\boldsymbol{Q}(\boldsymbol{x}-\boldsymbol{\mu})_{=q}$$

If **x** is sampled, then

$$q = \mathbf{z}^T \mathbf{z}$$

otherwise, compute this term as

•
$$\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{\mu}$$

•
$$q = \mathbf{u}^T \mathbf{v}$$

The log-density is

$$\log \pi(\boldsymbol{x}) = -\frac{n}{2}\log 2\pi + \sum_{i=1}^{n}\log L_{ii} - \frac{1}{2}(\underbrace{\boldsymbol{x}-\boldsymbol{\mu}})^{T}\boldsymbol{Q}(\boldsymbol{x}-\boldsymbol{\mu})_{=q}$$

If **x** is sampled, then

$$q = \mathbf{z}^T \mathbf{z}$$

otherwise, compute this term as

•
$$\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{\mu}$$

•
$$q = \boldsymbol{u}^T \boldsymbol{v}$$

3 1 4 3
Part IV

Numerical methods for sparse matrices

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 47 / 135

Numerical methods for sparse matrices



Computations on GMRFs can be expressed such that the main tasks are

- compute the Cholesky factorisation of $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$, and
- 2 solve Lv = b and $L^T x = z$.
- The second task is much-faster than the first, but sparsity will be of advantage also here.

Numerical methods for sparse matrices



Computations on GMRFs can be expressed such that the main tasks are

- compute the Cholesky factorisation of $Q = LL^T$, and
- **2** solve Lv = b and $L^T x = z$.
- The second task is much-faster than the first, but sparsity will be of advantage also here.

Numerical methods for sparse matrices



Computations on GMRFs can be expressed such that the main tasks are

- compute the Cholesky factorisation of $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$, and
- **2** solve Lv = b and $L^T x = z$.
- The second task is much-faster than the first, but sparsity will be of advantage also here.

The questions are

• why a sparse Q allow for fast factorisation,

- how we can take advantage of it,
- why we gain if we permute the vertics before factorising the matrix

The questions are

- why a sparse Q allow for fast factorisation,
- how we can take advantage of it,
- why we gain if we permute the vertics before factorising the matrix

The questions are

- why a sparse Q allow for fast factorisation,
- how we can take advantage of it,
- why we gain if we permute the vertics before factorising the matrix

How to compute the Cholesky factorisation



$$\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$$
$$Q_{ij} = \sum_{k=1}^{j} L_{ik}L_{jk}, \qquad \mathbf{v}_{i} = Q_{ij} - \sum_{k=1}^{j-1} L_{ik}L_{jk}, \quad i \geq j,$$

Then

• $L_{jj}^2 = v_j$, and • $L_{ij}L_{jj} = v_i$ for i > j.

If we know $\{v_i\}$ for fixed *j*, then

$$L_{jj} = \sqrt{v_j}$$
 and $L_{ij} = v_i/\sqrt{v_j}$, for $i = j + 1, \dots, n$.

This gives the *j*th column in **L**.

E ● E ● ○ Q C Oct 2018 50 / 135

F 4 3 F 4 3 F

How to compute the Cholesky factorisation



$$\boldsymbol{Q} = \boldsymbol{L}\boldsymbol{L}^{T}$$
$$Q_{ij} = \sum_{k=1}^{j} L_{ik}L_{jk}, \qquad v_{i} = Q_{ij} - \sum_{k=1}^{j-1} L_{ik}L_{jk}, \quad i \geq j,$$

Then

If we know $\{v_i\}$ for fixed *j*, then

$$L_{jj} = \sqrt{v_j}$$
 and $L_{ij} = v_i/\sqrt{v_j}$, for $i = j + 1, \dots, n$.

This gives the *j*th column in **L**.

Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 50 / 135

▶ ∢ ⊒

How to compute the Cholesky factorisation



$$\boldsymbol{Q} = \boldsymbol{L}\boldsymbol{L}^{T}$$
$$Q_{ij} = \sum_{k=1}^{j} L_{ik}L_{jk}, \qquad v_i = Q_{ij} - \sum_{k=1}^{j-1} L_{ik}L_{jk}, \quad i \geq j,$$

Then

• $L_{jj}^2 = v_j$, and • $L_{ij}L_{jj} = v_i$ for i > j.

If we know $\{v_i\}$ for fixed *j*, then

$$L_{jj} = \sqrt{v_j}$$
 and $L_{ij} = v_i/\sqrt{v_j}$, for $i = j + 1, \dots, n$.

This gives the *j*th column in *L*.

→ ∢ ≣

Cholesky factorization of $\mathbf{Q} > 0$

Algorithm 4 Computing the Cholesky triangle L of Q

- 1: **for** j = 1 **to** n **do**
- 2: $v_{j:n} = Q_{j:n,j}$
- 3: **for** k = 1 **to** j 1 **do** $v_{j:n} = v_{j:n} L_{j:n,k}L_{jk}$
- 4: $L_{j:n,j} = v_{j:n}/\sqrt{v_j}$
- 5: **end for**
- 6: Return *L*

The overall process involves $n^3/3$ flops.

(4 間) トイヨト イヨト



Interpretation of *L* (I)



$$\boldsymbol{L}^T \boldsymbol{x} = \boldsymbol{z}$$
 where $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$

is $\mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}^{-1})$ distributed.

Since *L* is lower triangular then

$$x_{n} = \frac{1}{L_{nn}} z_{n}$$
$$x_{n-1} = \frac{1}{L_{n-1,n-1}} \left(z_{n-1} - L_{n,n-1} x_{n} \right)$$





Oct 2018 52 / 135

3 1 4 3

Interpretation of *L* (I)

Let $\boldsymbol{Q} = \boldsymbol{L}\boldsymbol{L}^{T}$, then the solution of

$$\boldsymbol{L}^{T}\boldsymbol{x} = \boldsymbol{z}$$
 where $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$

. . .

is $\mathcal{N}(\boldsymbol{0}, \boldsymbol{Q}^{-1})$ distributed.

Since *L* is lower triangular then

$$x_{n} = \frac{1}{L_{nn}} z_{n}$$
$$x_{n-1} = \frac{1}{L_{n-1,n-1}} (z_{n-1} - L_{n,n-1} x_{n})$$





Interpretation of *L* (II)



Theorem

Let **x** be a GMRF wrt to the labelled graph G, with mean **0** and precision matrix $\mathbf{Q} > 0$. Let **L** be the Cholesky triangle of **Q**. Then for $i \in \mathcal{V}$,

$$E(x_i \mid \boldsymbol{x}_{(i+1):n}) = -\frac{1}{L_{ii}} \sum_{j=i+1}^n L_{ji} x_j \quad and$$
$$Prec(x_i \mid \boldsymbol{x}_{(i+1):n}) = L_{ii}^2.$$

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 53 / 135

3 🖌 🖌 3

Determine the zero-pattern in \boldsymbol{L} (I)



Theorem

Let **x** be a GMRF wrt \mathcal{G} , with mean **0** and precision matrix **Q** > 0. Let **L** be the Cholesky triangle of **Q** and define for $1 \le i < j \le n$ the set

$$F(i,j) = \{i+1,\ldots,j-1,j+1,\ldots,n\},\$$

which is the future of i except j. Then

$$x_i \perp x_j \mid \mathbf{x}_{F(i,j)} \iff L_{ji} = 0.$$

Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 54 / 135

ヨトィヨト



Theorem

Let **x** be a GMRF wrt *G*, with mean **0** and precision matrix **Q** > 0. Let **L** be the Cholesky triangle of **Q** and define for $1 \le i < j \le n$ the set

$$F(i,j) = \{i + 1, \dots, j - 1, j + 1, \dots, n\},\$$

which is the future of i except j. Then

$$x_i \perp x_j \mid \mathbf{x}_{F(i,j)} \iff L_{ji} = 0.$$

If we can verify that L_{ii} is zero, we do not have to compute it when factorising **Q**

Håvard Rue (haavard.rue@kaust.edu.sa)

Proof



Assume $\mu = \mathbf{0}$ and fix $1 \le i < j \le n$. Theorem 3 gives that

$$\pi(\mathbf{x}_{i:n}) \propto \exp\left(-\frac{1}{2}\sum_{k=i}^{n}L_{kk}^{2}\left(x_{k}+\frac{1}{L_{kk}}\sum_{j=k+1}^{n}L_{jk}x_{j}\right)^{2}\right)$$
$$= \exp\left(-\frac{1}{2}\mathbf{x}_{i:n}^{T}\mathbf{Q}^{(i:n)}\mathbf{x}_{i:n}\right),$$

where $Q_{ij}^{(i:n)} = L_{ii}L_{ji}$. Then

$$x_i \perp x_j \mid \mathbf{x}_{F(i,j)} \quad \Longleftrightarrow \quad L_{ii}L_{ji} = 0,$$

which is equivalent to $L_{ji} = 0$ since $L_{ii} > 0$ as $\mathbf{Q}^{(i:n)} > 0$.

Proof



Assume $\mu = \mathbf{0}$ and fix $1 \le i < j \le n$. Theorem 3 gives that

$$\pi(\boldsymbol{x}_{i:n}) \propto \exp\left(-\frac{1}{2}\sum_{k=i}^{n}L_{kk}^{2}\left(x_{k}+\frac{1}{L_{kk}}\sum_{j=k+1}^{n}L_{jk}x_{j}\right)^{2}\right)$$
$$= \exp\left(-\frac{1}{2}\boldsymbol{x}_{i:n}^{T}\boldsymbol{Q}^{(i:n)}\boldsymbol{x}_{i:n}\right),$$

where $Q_{ij}^{(i:n)} = L_{ii}L_{ji}$. Then

$$x_i \perp x_j \mid \mathbf{x}_{F(i,j)} \iff L_{ii}L_{ji} = 0,$$

which is equivalent to $L_{ji} = 0$ since $L_{ii} > 0$ as $\mathbf{Q}^{(i:n)} > 0$.

◆□▶★録▶★国▶★国▶ = 国

(Global Markov property)

Let \mathbf{x} be a GMRF wrt $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. The global Markov property:

$$\mathbf{x}_A \perp \mathbf{x}_B \mid \mathbf{x}_C$$

for all disjoint sets *A*, *B* and *C* where *C* separates *A* and *B*, and *A* and *B* are non-empty.







The **global Markov property** provide a simple and sufficient criteria for checking if $L_{ji} = 0$.

Corollary

If F(i, j) separates i < j in \mathcal{G} , then $L_{ji} = 0$.

Corollary

If $i \sim j$ then F(i, j) does not separates i < j.

The idea is simple

- Use the global Markov property to check if $L_{jj} = 0$.
- Compute only the non-zero terms in L, so that $Q = LL^T$.



The global Markov property provide a simple and sufficient criteria for checking if $L_{ii} = 0$.

Corollary

If F(i, j) separates i < j in \mathcal{G} , then $L_{ii} = 0$.

- Compute only the non-zero terms in L, so that $Q = LL^{T}$.



The global Markov property provide a simple and sufficient criteria for checking if $L_{ii} = 0$.

Corollary

If F(i, j) separates i < j in \mathcal{G} , then $L_{ii} = 0$.

Corollary

If $i \sim j$ then F(i, j) does not separates i < j.

- Compute only the non-zero terms in L, so that $Q = LL^{T}$.



The **global Markov property** provide a simple and sufficient criteria for checking if $L_{ji} = 0$.

Corollary

If F(i, j) separates i < j in G, then $L_{ji} = 0$.

Corollary

If $i \sim j$ then F(i, j) does not separates i < j.

The idea is simple

- Use the *global Markov property* to check if $L_{ji} = 0$.
- Compute only the non-zero terms in \boldsymbol{L} , so that $\boldsymbol{Q} = \boldsymbol{L} \boldsymbol{L}^{T}$.





E ► E • つ Q C Oct 2018 58 / 135

(4 間) トイヨト イヨト





E ► E • つ Q C Oct 2018 58 / 135

▶ ★ 臣 ▶ ★ 臣





E ● E のQC Oct 2018 58 / 135

とくきとくき





E ≥ ● Q C Oct 2018 59 / 135

とくきとくき

Example: AR(1)-process





$$x_t \mid \mathbf{x}_{1:(t-1)} \sim \mathcal{N}(\phi x_{t-1}, \sigma^2), \quad t = 1, \dots, n$$



Example: AR(1)-process





.

Example: AR(1)-process



イロト イヨト イヨト

Bandwidth is preserved



Similarly, for an AR(p)-process

- **Q** have bandwidth *p*.
- L have lower-bandwidth p.

Theorem

Let **Q** > 0 be a band matrix with bandwidth p and dimension n, then the Cholesky triangle of **Q** has (lower) bandwidth p.

...easy to modify existing Cholesky-factorisation code to use only entries where $|i - j| \le p$.

Håvard Rue (haavard.rue@kaust.edu.sa)

Bandwidth is preserved

Similarly, for an AR(p)-process

- **Q** have bandwidth *p*.
- L have lower-bandwidth p.

Theorem

Let $\mathbf{Q} > 0$ be a band matrix with bandwidth p and dimension n, then the Cholesky triangle of **Q** has (lower) bandwidth p.



イロト イポト イヨト イヨ

Håvard Rue (haavard.rue@kaust.edu.sa)

Bandwidth is preserved

Bandwidth is preserved

Similarly, for an AR(p)-process

- **Q** have bandwidth *p*.
- L have lower-bandwidth p.

Theorem

Let $\mathbf{Q} > 0$ be a band matrix with bandwidth p and dimension n, then the Cholesky triangle of **Q** has (lower) bandwidth p.



...easy to modify existing Cholesky-factorisation code to use only entries where |i - j| < p. イロト イポト イヨト イヨ

Håvard Rue (haavard.rue@kaust.edu.sa)

bavescomp.kaust.edu.sa

Oct 2018 61 / 135

Reorder the vertices



We can permute the vertexes;

select one of the n! possible permutations, define the corresponding permutation matrix **P**, such that $\mathbf{i}^{P} = \mathbf{P}\mathbf{i}$, where $\mathbf{i} = (1, ..., n)^{T}$, is the new ordering of the vertexes.

Chose **P**, if possible, such that

$$\mathbf{Q}^{P} = \mathbf{P}\mathbf{Q}\mathbf{P}^{T} \tag{3}$$

is a band-matrix with a small bandwidth.

Reorder the vertices



We can permute the vertexes;

select one of the n! possible permutations, define the corresponding permutation matrix **P**, such that $\mathbf{i}^{P} = \mathbf{P}\mathbf{i}$, where $\mathbf{i} = (1, ..., n)^{T}$, is the new ordering of the vertexes.

Chose P, if possible, such that

$$\mathbf{Q}^{P} = \mathbf{P}\mathbf{Q}\mathbf{P}^{T}$$
(3)

is a band-matrix with a small bandwidth.

• Impossible in general to obtain the optimal permutation, *n*! is to large!

- A sub-optimal ordering will do as well.
- Solve $Q\mu = b$ as follows:
 - $\boldsymbol{b}^{P} = \boldsymbol{P}\boldsymbol{b}.$
 - Solve $\boldsymbol{Q}^{P}\boldsymbol{\mu}^{P}=\boldsymbol{b}^{P}$
 - Map the solution back, $\boldsymbol{\mu} = \boldsymbol{P}^T \boldsymbol{\mu}^P$.
• Impossible in general to obtain the optimal permutation, *n*! is to large!

- A sub-optimal ordering will do as well.
- Solve $Q\mu = b$ as follows:

•
$$\boldsymbol{b}^{P} = \boldsymbol{P}\boldsymbol{b}.$$

• Solve
$$\boldsymbol{Q}^P \boldsymbol{\mu}^P = \boldsymbol{b}^P$$

• Map the solution back, $\boldsymbol{\mu} = \boldsymbol{P}^T \boldsymbol{\mu}^P$.

(日)

- Impossible in general to obtain the optimal permutation, *n*! is to large!
- A sub-optimal ordering will do as well.
- Solve $oldsymbol{Q} oldsymbol{\mu} = oldsymbol{b}$ as follows:
 - $\boldsymbol{b}^{P} = \boldsymbol{P}\boldsymbol{b}.$
 - Solve $\boldsymbol{Q}^{P}\boldsymbol{\mu}^{P}=\boldsymbol{b}^{P}$
 - Map the solution back, $\boldsymbol{\mu} = \boldsymbol{P}^T \boldsymbol{\mu}^P$.

(

Reordering to band-matrices



Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 64 / 135

(

Reordering to band-matrices





Reordering to band-matrices



Oct 2018 66 / 135



























The idea generalise as follows.

- Select a (small) set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size.
- Order the nodes chosen *after* ordering all the nodes in both subgraphs.
- Apply this procedure recursively to the nodes in each subgraph.
- Costs in the spatial case
 - Factorisation $\mathcal{O}(n^{3/2})$
 - Fill-in *O*(*n* log *n*)
 - Optimal in the order sense.



The idea generalise as follows.

- Select a (small) set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size.
- Order the nodes chosen *after* ordering all the nodes in both subgraphs.
- Apply this procedure recursively to the nodes in each subgraph.

- Factorisation 𝒪(n^{3/2})
- Fill-in $\mathcal{O}(n \log n)$
- Optimal in the order sense.



The idea generalise as follows.

- Select a (small) set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size.
- Order the nodes chosen *after* ordering all the nodes in both subgraphs.
- Apply this procedure recursively to the nodes in each subgraph.

- Factorisation O(n^{3/2})
- Fill-in $\mathcal{O}(n \log n)$
- Optimal in the order sense.



The idea generalise as follows.

- Select a (small) set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size.
- Order the nodes chosen *after* ordering all the nodes in both subgraphs.
- Apply this procedure recursively to the nodes in each subgraph.

- Factorisation O(n^{3/2})
- Fill-in $\mathcal{O}(n \log n)$
- Optimal in the order sense.



The idea generalise as follows.

- Select a (small) set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size.
- Order the nodes chosen *after* ordering all the nodes in both subgraphs.
- Apply this procedure recursively to the nodes in each subgraph.

- Factorisation $\mathcal{O}(n^{3/2})$
- Fill-in $\mathcal{O}(n \log n)$
- Optimal in the order sense.



The idea generalise as follows.

- Select a (small) set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size.
- Order the nodes chosen *after* ordering all the nodes in both subgraphs.
- Apply this procedure recursively to the nodes in each subgraph.

- Factorisation $\mathcal{O}(n^{3/2})$
- Fill-in $\mathcal{O}(n \log n)$
- Optimal in the order sense.



The idea generalise as follows.

- Select a (small) set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size.
- Order the nodes chosen *after* ordering all the nodes in both subgraphs.
- Apply this procedure recursively to the nodes in each subgraph.

- Factorisation $\mathcal{O}(n^{3/2})$
- Fill-in $\mathcal{O}(n \log n)$
- Optimal in the order sense.





Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 69 / 135

ģ

Nested dissection reordering (II)





Oct 2018 69 / 135





・ロト・日本・ キョン・ 日本

How to deal with sparse matrices?



- Use existing software.
- In R use (recomended) package Matrix, create sparse matrices with sparseMatrix() etc...

Part V

Marginal variance

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 71 / 135

3 1 4 3



Computing marginal variances for GMRFs*

Let

$$Q = V D V^7$$

- where **D** is a diagonal matrix, and
- **V** is a lower triangular matrix with ones on the diagonal.

The matrix identity

 $\boldsymbol{\Sigma} = \boldsymbol{D}^{-1} \boldsymbol{V}^{-1} + (\boldsymbol{I} - \boldsymbol{V}^{T}) \boldsymbol{\Sigma}$

define recursions which can be used to compute

• Var(x_i) and Cov(x_i, x_j) for $i \sim j$

essentially without cost when the Cholesky triangle **L** is known (TFC '73).

(日)



Computing marginal variances for GMRFs*

Let

$$Q = V D V^7$$

• where **D** is a diagonal matrix, and

• **V** is a lower triangular matrix with ones on the diagonal. The matrix identity

$$\boldsymbol{\Sigma} = \boldsymbol{D}^{-1} \boldsymbol{V}^{-1} + (\boldsymbol{I} - \boldsymbol{V}^T) \boldsymbol{\Sigma}$$

define recursions which can be used to compute

• Var(x_i) and Cov(x_i, x_j) for $i \sim j$

essentially without cost when the Cholesky triangle *L* is known (TFC '73).

FORMATION OF A SPARSE BUS IMPEDANCE MATRIX AND ITS APPLICATION TO SHORT CIRCUIT STUDY

by

Kazuhiro Takahashi, John Fagan and Mo-Shing Chen

ABSTRACT

This paper proposes a new computational method for the formation of a sparse bus impedance matrix. An algorithm is introduced which generates only the relevant terms of the bus impedance matrix for short circuit calculation. The algorithm is presented as it applies to the solution of short circuit problems. The method offers a decrease in execution time and a reduction in core memory requirements for the digital computer. These advantages are superior to conventional methods of short circuit calculation such as the ordinary Z matrix and the factorized Y matrix methods.

A small sample system is provided to illustrate the computational procedure. Application to practical large power systems has been proven by the development of a digital computer program based upon the proposed method.

The following considerations are made to extend the method for more practical usage; 1) Mutual coupling of transmission lines, 2) Short circuit currents more than 2 busses away, 3) Asymmetric fault analysis, 4) Modification of the matrix elements due to the network configuration change, and 5) Inversion of asymmetric sparse matrix.

$$I_{ss} = 1/Z_{ss}$$
(1)
$$I_{st} = I_{ss} \cdot (Z_{ss} - Z_{st})/\mathcal{J}_{st}$$
(2)

where I_{SS} is the three phase short circuit current at the faulted bus s

 $\mathbf{I}_{\texttt{st}}$ is the current of the connecting line (st) due to the fault

 \mathfrak{F}_{st} is the impedance of the connecting line (st) \mathbf{Z}_{ss} is the driving point impedance at the faulted bus s

 \mathbf{Z}_{st} is the transfer impedance of the faulted bus s to the adjacent bus t

These system parameters are normally complex. However, real numbers are used in this paper to illustrate the method.

The driving point and transfer impedances given in eqs. (1) and (2) are normally obtained by calculating all the terms of the bus impedance matrix. The bus impedance matrix, or simply Z matrix, is defined by the inverse of the bus admittance matrix Y. Both matrices are symmetric. The Y matrix is generally sparse for practical power systems while the Z matrix is full.

A small DC network is provided in Fig. 2, which

• □ ▶ • □ ▶ • □ ▶ • □ ▶ • □ ▶

Statistical derivation



Recall for a zero mean GMRF that

$$x_i \mid x_{i+1}, \ldots, x_n \sim \mathcal{N}(-\frac{1}{L_{ii}}\sum_{k=i+1}^n L_{ki}x_k, 1/L_{ii}^2), \quad i=n,\ldots,1.$$

provides a sequential representation of the GMRF backward in "time" i.

Multiply by x_j , $j \ge i$, and taking expectation yields

$$\Sigma_{ij} = \delta_{ij}/L_{ii}^2 - \frac{1}{L_{ii}}\sum_{k\in\mathcal{I}(i)}^n L_{ki}\Sigma_{kj}, \quad j\geq i, \ i=n,\ldots,1,$$

where $\mathcal{I}(i)$ as those k where L_{ki} is non-zero,

$$\mathcal{I}(i) = \{k > i : L_{ki} \neq 0\}$$

and δ_{ij} is one if i = j and zero otherwise.

F 4 3 F 4 3 F

We can use

$$\Sigma_{ij} = \delta_{ij}/L_{ii}^2 - \frac{1}{L_{ii}}\sum_{k\in\mathcal{I}(i)}^n L_{ki}\Sigma_{kj}, \quad j\geq i, \ i=n,\ldots,1,$$

to compute Σ_{ij} for each ij:

- Outer loop $i = n, \ldots, 1$
- Inner loop $j = n, \ldots, i$

• • = • • = •

Example

Let n = 3, $\mathcal{I}(1) = \{2, 3\}$, $\mathcal{I}(2) = \{3\}$, then we get

$$\begin{split} \Sigma_{33} &= \frac{1}{L_{33}^2} & \Sigma_{23} = -\frac{1}{L_{22}} \left(L_{32} \Sigma_{33} \right) \\ \Sigma_{22} &= \frac{1}{L_{22}^2} - \frac{1}{L_{22}} \left(L_{32} \Sigma_{32} \right) & \Sigma_{13} = -\frac{1}{L_{11}} \left(L_{21} \Sigma_{23} + L_{31} \Sigma_{33} \right) \\ \Sigma_{12} &= -\frac{1}{L_{11}} \left(L_{21} \Sigma_{22} + L_{31} \Sigma_{32} \right) & \Sigma_{11} = \frac{1}{L_{11}^2} - \frac{1}{L_{11}} \left(L_{21} \Sigma_{21} + L_{31} \Sigma_{31} \right) \end{split}$$

where we also need to use that Σ is symmetric.

3 1 4 3

• Assume we want to compute all marginal variances.

- To do so, we need to compute Σ_{ij} (or Σ_{ji}) for all *ij* in some set S.
- If the recursions can be solved by only computing Σ_{ij} for all $ij \in S$ we say that the recursions are *solvable* using S.

3 🕨 🖌 3

- Assume we want to compute all marginal variances.
- To do so, we need to compute Σ_{ij} (or Σ_{ji}) for all ij in some set S.
- If the recursions can be solved by only computing Σ_{ij} for all $ij \in S$ we say that the recursions are *solvable* using S.

ヨト・モラト

- Assume we want to compute all marginal variances.
- To do so, we need to compute Σ_{ij} (or Σ_{ji}) for all ij in some set S.
- If the recursions can be solved by only computing Σ_{ij} for all $ij \in S$ we say that the recursions are *solvable* using S.

From

$$\Sigma_{ij} = \delta_{ij}/L_{ii}^2 - \frac{1}{L_{ii}}\sum_{k\in\mathcal{I}(i)}^n L_{ki}\Sigma_{kj}, \quad j\geq i, \ i=n,\ldots,1,$$
(4)

it is evident that $\mathcal S$ must satisfy

$$ij \in S$$
 and $k \in \mathcal{I}(i) \longrightarrow kj \in S$ (5)

we also need that $ii \in S$ for $i = 1, \ldots, n$.

◆ロト ◆聞ト ◆臣ト ◆臣ト

From

$$\Sigma_{ij} = \delta_{ij}/L_{ii}^2 - \frac{1}{L_{ii}}\sum_{k\in\mathcal{I}(i)}^n L_{ki}\Sigma_{kj}, \quad j\geq i, \ i=n,\ldots,1,$$
(4)

it is evident that $\mathcal S$ must satisfy

$$ij \in S$$
 and $k \in \mathcal{I}(i) \longrightarrow kj \in S$ (5)

we also need that $ii \in S$ for $i = 1, \ldots, n$.

F 4 3 F 4 3 F

- $S = V \times V$ is a valid set, but we want |S| to be small to avoid unnecessary computations.
- a minimal set depends however on the numerical values in *L*, or *Q* implicitly.
- a slightly larger set, that contains the minimal, turn out to be the one used to compute *L*!!!

Theorem (TFC'73)

 $S = \{ij \in \mathcal{V} \times \mathcal{V} : j \ge i, i \text{ and } j \text{ are not separated by } F(i, j)\}$

is solvable.
- $S = V \times V$ is a valid set, but we want |S| to be small to avoid unnecessary computations.
- a minimal set depends however on the numerical values in *L*, or *Q* implicitly.
- a slightly larger set, that contains the minimal, turn out to be the one used to compute *L*!!!

Theorem (TFC'73)

 $S = \{ij \in \mathcal{V} \times \mathcal{V} : j \ge i, i \text{ and } j \text{ are not separated by } F(i, j)\}$

is solvable.

- $S = V \times V$ is a valid set, but we want |S| to be small to avoid unnecessary computations.
- a minimal set depends however on the numerical values in *L*, or *Q* implicitly.
- a slightly larger set, that contains the minimal, turn out to be the one used to compute *L*!!!

Theorem (TFC'73)

 $S = \{ij \in \mathcal{V} \times \mathcal{V} : j \ge i, i \text{ and } j \text{ are not separated by } F(i,j)\}$

is solvable.

イロト イポト イヨト イヨト

- $S = V \times V$ is a valid set, but we want |S| to be small to avoid unnecessary computations.
- a minimal set depends however on the numerical values in *L*, or *Q* implicitly.
- a slightly larger set, that contains the minimal, turn out to be the one used to compute *L*!!!

Theorem (TFC'73)

 $S = \{ij \in V \times V : j \ge i, i \text{ and } j \text{ are not separated by } F(i,j)\}$

is solvable.

• • = • • = •

Main idea of the proof:



$ij \in S$ and $k \in \mathcal{I}(i) \longrightarrow kj \in S$, i < j, k < j (6)

• $ij \in S$, says there is a path from *i* to *j* where all nodes $\leq i$.

- $k \in \mathcal{I}(i)$, says there is path from *i* to *k* where all nodes $\leq i$.
- then there must be some path from k to i to j where all nodes are ≤ i, hence kj ∈ S.

・ロト ・ 母 ト ・ ヨ ト ・ ヨ ト

Main idea of the proof:



$$ij \in S$$
 and $k \in \mathcal{I}(i) \longrightarrow kj \in S$, $i < j$, $k < j$ (6)

- $ij \in S$, says there is a path from *i* to *j* where all nodes $\leq i$.
- $k \in \mathcal{I}(i)$, says there is path from *i* to *k* where all nodes $\leq i$.
- then there must be some path from k to i to j where all nodes are ≤ i, hence kj ∈ S.

Main idea of the proof:



$$ij \in S$$
 and $k \in \mathcal{I}(i) \longrightarrow kj \in S$, $i < j$, $k < j$ (6)

- $ij \in S$, says there is a path from *i* to *j* where all nodes $\leq i$.
- $k \in \mathcal{I}(i)$, says there is path from *i* to *k* where all nodes $\leq i$.
- then there must be some path from k to i to j where all nodes are ≤ i, hence kj ∈ S.

Interpretation of \mathcal{S}



• S is the set of all possible non-zero elements in L based on G only.

- this is the set of L_{ii} 's that are computed when computing $Q = LL^T$.
- since $L_{ji} \neq 0$ in general when $i \sim j$, then we compute also $Cov(x_i, x_j)$ for $i \sim j$.
- some of the L_{ij}'s might turn out to be zero depending on the conditional independence properties of the marginal density for x_{i:n} for i = n, ..., 1.

イロト イヨト イヨト

Interpretation of \mathcal{S}



- S is the set of all possible non-zero elements in L based on G only.
- this is the set of L_{ji} 's that are computed when computing $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$.
- since $L_{ji} \neq 0$ in general when $i \sim j$, then we compute also $Cov(x_i, x_j)$ for $i \sim j$.
- some of the L_{ij}'s might turn out to be zero depending on the conditional independence properties of the marginal density for x_{i:n} for i = n, ..., 1.

(日)

Interpretation of \mathcal{S}



- S is the set of all possible non-zero elements in L based on G only.
- this is the set of L_{ji} 's that are computed when computing $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$.
- since $L_{ji} \neq 0$ in general when $i \sim j$, then we compute also $Cov(x_i, x_j)$ for $i \sim j$.
- some of the L_{ij}'s might turn out to be zero depending on the conditional independence properties of the marginal density for x_{i:n} for i = n, ..., 1.

(日)

Interpretation of $\mathcal S$

- S is the set of all possible non-zero elements in L based on G only.
- this is the set of L_{ji} 's that are computed when computing $\mathbf{Q} = \mathbf{L}\mathbf{L}^{T}$.
- since $L_{ji} \neq 0$ in general when $i \sim j$, then we compute also $Cov(x_i, x_j)$ for $i \sim j$.
- some of the L_{ij}'s might turn out to be zero depending on the conditional independence properties of the marginal density for x_{i:n} for i = n, ..., 1.

General algorithm



for i = n, ..., 1for decreasing j in $\mathcal{I}(i)$ compute Σ_{ij} from eq. (4)

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

E ► E • つ Q C Oct 2018 83 / 135

• 3 > 4 3

band matrices



for
$$i = n, ..., 1$$

for $j = \min(i + b_w, n), ..., i$
compute Σ_{ij} from eq. (4).

equivalent to Kalman-recursions for smoothing.

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

● E つへで
 Oct 2018 84 / 135

• • = • • =

Part VI

INLA

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

・ E うへの
 Oct 2018 85 / 135

イロト イポト イヨト イヨト

Latent Gaussian models is a model of the following form

- Observed data $\boldsymbol{y}, y_i | x_i \sim \pi(y_i | x_i, \boldsymbol{\theta})$
- Latent Gaussian field $m{x} \sim \mathcal{N}(\cdot, m{Q}(m{ heta})^{-1})$
- Hyperparameters θ
 - variability
 - length/strength of dependence
 - parameters in the likelihood

$$\pi(\boldsymbol{x}, \boldsymbol{\theta} \mid \boldsymbol{y}) \propto \pi(\boldsymbol{\theta}) \ \pi(\boldsymbol{x} \mid \boldsymbol{\theta}) \prod_{i \in \mathcal{I}} \pi(y_i \mid x_i, \boldsymbol{\theta})$$



Oct 2018 86 / 135

F 4 3 F 4 3 F

Latent Gaussian models is a model of the following form

- Observed data $\boldsymbol{y}, y_i | x_i \sim \pi(y_i | x_i, \boldsymbol{\theta})$
- Latent Gaussian field $\pmb{x} \sim \mathcal{N}(\cdot, \pmb{Q}(\pmb{ heta})^{-1})$
- Hyperparameters θ
 - variability
 - length/strength of dependence
 - parameters in the likelihood

$$\pi(\mathbf{x}, \boldsymbol{\theta} \mid \mathbf{y}) \propto \pi(\boldsymbol{\theta}) \ \pi(\mathbf{x} \mid \boldsymbol{\theta}) \prod_{i \in \mathcal{I}} \pi(y_i \mid x_i, \boldsymbol{\theta})$$



Oct 2018 86 / 135

Latent Gaussian models is a model of the following form

- Observed data $\boldsymbol{y}, y_i | x_i \sim \pi(y_i | x_i, \boldsymbol{\theta})$
- Latent Gaussian field $\pmb{x} \sim \mathcal{N}(\cdot, \pmb{Q}(\pmb{ heta})^{-1})$
- Hyperparameters θ
 - variability
 - length/strength of dependence
 - parameters in the likelihood

$$\pi(\boldsymbol{x}, \boldsymbol{\theta} \mid \boldsymbol{y}) \propto \pi(\boldsymbol{\theta}) \ \pi(\boldsymbol{x} \mid \boldsymbol{\theta}) \prod_{i \in \mathcal{I}} \pi(y_i \mid x_i, \boldsymbol{\theta})$$



Oct 2018 86 / 135

Latent Gaussian models is a model of the following form

- Observed data $\boldsymbol{y}, y_i | x_i \sim \pi(y_i | x_i, \boldsymbol{\theta})$
- Latent Gaussian field $\pmb{x} \sim \mathcal{N}(\cdot, \pmb{Q}(\pmb{ heta})^{-1})$
- Hyperparameters θ
 - variability
 - length/strength of dependence
 - parameters in the likelihood

$$\pi(\mathbf{x}, \mathbf{\theta} \mid \mathbf{y}) \propto \pi(\mathbf{\theta}) \ \pi(\mathbf{x} \mid \mathbf{\theta}) \prod_{i \in \mathcal{I}} \pi(y_i \mid x_i, \mathbf{\theta})$$



Oct 2018 86 / 135



Compute from

$$\pi(\mathbf{x}, \mathbf{\theta} \mid \mathbf{y}) \propto \pi(\mathbf{\theta}) \ \pi(\mathbf{x} \mid \mathbf{\theta}) \prod_{i \in \mathcal{I}} \pi(y_i \mid x_i)$$

the posterior marginals:

 $\pi(x_i \mid \mathbf{y}),$ for some or all *i*

and/or

$$\pi(\theta_i \mid \mathbf{y}), \qquad ext{for some or all } i$$

3 1 4 3

Our approach: Approximate Bayesian Inference



• Can we compute (approximate) marginals directly without using MCMC?

- YES!
- Gain
 - Huge speedup & accuracy
 - The ability to treat latent Gaussian models properly ;-)

Our approach: Approximate Bayesian Inference



• Can we compute (approximate) marginals directly without using MCMC?

YES!

Gain

- Huge speedup & accuracy
- The ability to treat latent Gaussian models properly ;-)





- Can we compute (approximate) marginals directly without using MCMC?
- YES!
- Gain
 - Huge speedup & accuracy
 - The ability to treat latent Gaussian models properly ;-)

Smoothing noisy observations (I)



Observations

$$y_i = m(i) + \epsilon_i, \qquad i = 1, \ldots, n$$

for Gaussian iid noise ϵ_i with *known* precision.

Will assume *m*(*i*) is a smooth function wrt *i*

Smoothing noisy observations (I)



Observations

$$y_i = m(i) + \epsilon_i, \qquad i = 1, \ldots, n$$

for Gaussian iid noise ϵ_i with *known* precision.

Will assume m(i) is a smooth function wrt i

Smoothing noisy observations (II)





Smoothing noisy observations (III)

Likelihood Gaussian observations with known precision

$$y_i | x_i, \theta \sim \mathcal{N}(x_i, \tau_0)$$

Latent A Gaussian model for the smooth function²

$$\pi(\boldsymbol{x}|\theta) \propto \theta^{(n-2)/2} \exp\left(-\frac{\theta}{2} \sum_{i=2}^{n} (x_i - 2x_{i-1} + x_{i-2})^2\right)$$

Hyperparameter The smoothing parameter θ which we assign a $\Gamma(a, b)$ prior

 $\pi(heta) \propto heta^{a-1} \exp\left(-b heta
ight), \quad heta > \mathsf{0}$



(日)



Smoothing noisy observations (III)

Likelihood Gaussian observations with known precision

$$y_i | x_i, \theta \sim \mathcal{N}(x_i, \tau_0)$$

Latent A Gaussian model for the smooth function²

$$\pi(\mathbf{x}|\theta) \propto \theta^{(n-2)/2} \exp\left(-\frac{\theta}{2}\sum_{i=2}^n (x_i - 2x_{i-1} + x_{i-2})^2\right)$$

Hyperparameter The smoothing parameter θ which we assign a $\Gamma(a, b)$ prior

 $\pi(heta) \propto heta^{a-1} \exp\left(-b heta
ight), \quad heta > 0$

²model="rw2"

Håvard Rue (haavard.rue@kaust.edu.sa)

(日)



Smoothing noisy observations (III)

Likelihood Gaussian observations with known precision

$$y_i | x_i, \theta \sim \mathcal{N}(x_i, \tau_0)$$

Latent A Gaussian model for the smooth function²

$$\pi(\mathbf{x}|\theta) \propto \theta^{(n-2)/2} \exp\left(-\frac{\theta}{2}\sum_{i=2}^n (x_i - 2x_{i-1} + x_{i-2})^2\right)$$

Hyperparameter The smoothing parameter θ which we assign a $\Gamma(a, b)$ prior

$$\pi(heta) \propto heta^{a-1} \exp\left(-b heta
ight), \quad heta > \mathsf{0}$$

²model="rw2"



Smoothing noisy observations (IV)



Since

$$oldsymbol{x},oldsymbol{y}| heta~\sim~\mathcal{N}(\cdot,\cdot)$$

we can compute (numerically) all marginals, using that



(人間) とうり くうり

Smoothing noisy observations (IV)



Since

$$oldsymbol{x},oldsymbol{y}| heta~\sim~\mathcal{N}(\cdot,\cdot)$$

we can compute (numerically) all marginals, using that





Posterior marginal for theta

▶ ★ 王



Posterior marginal for theta, interpolated

(Ξ) Ξ · ○ Q (○ Oct 2018 93 / 135

トイヨトイヨト

Smoothing noisy observations (V)



so that

 $oldsymbol{x}|oldsymbol{y}, heta~\sim~\mathcal{N}(\cdot,\cdot)$

$$\pi(x_i|\boldsymbol{y}) = \int \underbrace{\pi(x_i|\theta, \boldsymbol{y})}_{\text{Gaussian}} \pi(\theta|\boldsymbol{y}) \ d\theta$$

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

E ● E ● ○ Q C Oct 2018 94 / 135

◆ロト ◆聞 ト ◆ 国 ト ◆ 国 ト

Smoothing noisy observations (V)



$$oldsymbol{x}|oldsymbol{y}, heta~\sim~\mathcal{N}(\cdot,\cdot)$$

$$\pi(x_i|\boldsymbol{y}) = \int \underbrace{\pi(x_i|\theta, \boldsymbol{y})}_{\text{Gaussian}} \pi(\theta|\boldsymbol{y}) \ d\theta$$

Håvard Rue (haavard.rue@kaust.edu.sa)

E ● E ● ○ Q C Oct 2018 94 / 135

医子宫医子宫



Posterior marginal for theta

E Oct 2018 95 / 135

500

▶ < ≣ ▶



Posterior marginals for x[1] for each theta (unweighted)

Э Oct 2018 95 / 135

500

イロト イポト イヨト イヨト



Posterior marginals for x[1] for each theta (weighted)

х

イロト イポト イヨト イヨト
Posterior marginals for x[1]



Håvard Rue (haavard.rue@kaust.edu.sa)

< ■ ト ■ のへの Oct 2018 95 / 135

イロト イポト イヨト イヨト

Extensions



This is the basic idea behind INLA. It is really really simple.

However, we need to extend this basic idea so we can deal with
More than one hyperparameter
Non-Gaussian observations

Complications... Mostly practical

• • = • • =



This is the basic idea behind INLA. It is really really simple.

However, we need to extend this basic idea so we can deal with

- More than one hyperparameter
- Non-Gaussian observations
- Complications... Mostly practical

This is the basic idea behind INLA. It is really really simple.

Extensions

- More than one hyperparameter
- Non-Gaussian observations

Complications... Mostly practical



This is the basic idea behind INLA. It is really really simple.

Extensions

- More than one hyperparameter
- Non-Gaussian observations

Complications... Mostly practical



Extensions

This is the basic idea behind INLA. It is really really simple.

However, we need to extend this basic idea so we can deal with

- More than one hyperparameter
- Non-Gaussian observations

Complications... Mostly practical



More than one hyperparameter



Step I Explore $\pi(\theta|\mathbf{y})$

- Locate the mode
- Use the Hessian to construct new variables
- Grid-search

Step II From these integration points++, approximate the marginals for each θ_i

3 🕨 🖌 3

Extensions

More than one hyperparameter



Step I Explore $\pi(\theta|\mathbf{y})$

Locate the mode

- Use the Hessian to construct new variables
- Grid-search



More than one hyperparameter



Step I Explore $\pi(\theta|\mathbf{y})$

- Locate the mode
- Use the Hessian to construct new variables
- Grid-search

Step II From these integration points++, approximate the marginals for each θ_i



Oct 2018 97 / 135

More than one hyperparameter



Step I Explore $\pi(\theta|\mathbf{y})$

- Locate the mode
- Use the Hessian to construct new variables
- Grid-search

Step II From these integration points++, approximate the marginals for each θ_i



Oct 2018 97 / 135

Extensions

More than one hyperparameter



Step I Explore $\pi(\theta|\mathbf{y})$

- Locate the mode
- Use the Hessian to construct new variables
- Grid-search

Step II From these integration points++, approximate the marginals for each θ_i



Oct 2018 97 / 135

Non-Gaussian observations (I)



In this case



so we use an Gaussian approximation to the conditional

$$\pi(\theta|\mathbf{y}) \approx \operatorname{norm.const} \frac{\pi(\mathbf{x}, \mathbf{y}|\theta) \ \pi(\theta)}{\pi_{G}(\mathbf{x}|\mathbf{y}, \theta)} \bigg|_{x = \operatorname{xmode}(\theta)}$$

3 🕨 🖌 3

Non-Gaussian observations (I)



In this case



so we use an Gaussian approximation to the conditional

$$\pi(\theta|\mathbf{y}) \approx \operatorname{norm.const} \frac{\pi(\mathbf{x}, \mathbf{y}|\theta) \ \pi(\theta)}{\pi_{G}(\mathbf{x}|\mathbf{y}, \theta)} \bigg|_{x = \operatorname{xmode}(\theta)}$$

Non-Gaussian observations (II)

For the marginals for $x_i | \boldsymbol{y}, \boldsymbol{\theta}$, we do similarly

$$\pi(\mathbf{x}_i | \mathbf{y}, \boldsymbol{\theta}) \approx \operatorname{norm.const} \frac{\pi(\mathbf{x}, \mathbf{y} | \boldsymbol{\theta})}{\pi_G(\mathbf{x}_{-i} | \mathbf{x}_i, \mathbf{y}, \boldsymbol{\theta})} \bigg|_{\mathbf{x}_{-i} = \operatorname{xmode}(\boldsymbol{\theta}, \mathbf{x}_i)}$$

This is the hard part, as this is potentially very slow.



Non-Gaussian observations (II)

For the marginals for $x_i | \boldsymbol{y}, \boldsymbol{\theta}$, we do similarly

$$\pi(\mathbf{x}_i | \mathbf{y}, \boldsymbol{\theta}) \approx \operatorname{norm.const} \frac{\pi(\mathbf{x}, \mathbf{y} | \boldsymbol{\theta})}{\pi_G(\mathbf{x}_{-i} | \mathbf{x}_i, \mathbf{y}, \boldsymbol{\theta})} \bigg|_{\mathbf{x}_{-i} = \operatorname{xmode}(\boldsymbol{\theta}, \mathbf{x}_i)}$$

This is the hard part, as this is potentially very slow.



Main ideas (I)



Main ideas are simple and based on the identity

$$\pi(z) = rac{\pi(x,z)}{\pi(x|z)}$$
 leading to $\widetilde{\pi}(z) = rac{\pi(x,z)}{\widetilde{\pi}(x|z)}$

When $\tilde{\pi}(x|z)$ is the Gaussian-approximation, this is the Laplace-approximation.

Main ideas (I)



Main ideas are simple and based on the identity

$$\pi(z) = rac{\pi(x,z)}{\pi(x|z)}$$
 leading to $\widetilde{\pi}(z) = rac{\pi(x,z)}{\widetilde{\pi}(x|z)}$

When $\tilde{\pi}(x|z)$ is the Gaussian-approximation, this is the Laplace-approximation.

3 🕨 🖌 3

Main ideas (II)



Construct the approximations to

 $(\boldsymbol{\theta} | \boldsymbol{y})$ $\boldsymbol{\sigma}(\boldsymbol{x}_i | \boldsymbol{\theta}, \boldsymbol{y})$

then we integrate

$$egin{aligned} \pi(x_i|oldsymbol{y}) &= \int \pi(oldsymbol{ heta}|oldsymbol{y}) \; \pi(x_i|oldsymbol{ heta},oldsymbol{y}) \; doldsymbol{ heta} \ \pi(heta_j|oldsymbol{y}) &= \int \pi(oldsymbol{ heta}|oldsymbol{y}) \; doldsymbol{ heta}_{-j} \end{aligned}$$

◆ロト ◆聞 ト ◆ 国 ト ◆ 国 ト

Main ideas (II)



Construct the approximations to

- $\pi(\boldsymbol{\theta}|\boldsymbol{y})$
- 2 $\pi(x_i|\theta, y)$

then we integrate

$$egin{aligned} \pi(x_i|oldsymbol{y}) &= \int \pi(oldsymbol{ heta}|oldsymbol{y}) \; \pi(x_i|oldsymbol{ heta},oldsymbol{y}) \; doldsymbol{ heta} \ \pi(heta_j|oldsymbol{y}) &= \int \pi(oldsymbol{ heta}|oldsymbol{y}) \; doldsymbol{ heta}_{-j} \end{aligned}$$

ヨト・モラト

Main ideas (II)



Construct the approximations to

- $\pi(\boldsymbol{\theta}|\boldsymbol{y})$
- 2 $\pi(x_i|\theta, y)$

then we integrate

$$egin{aligned} \pi(x_i|oldsymbol{y}) &= \int \pi(oldsymbol{ heta}|oldsymbol{y}) \; \pi(x_i|oldsymbol{ heta},oldsymbol{y}) \; doldsymbol{ heta} \ \pi(heta_j|oldsymbol{y}) &= \int \pi(oldsymbol{ heta}|oldsymbol{y}) \; doldsymbol{ heta}_{-j} \end{aligned}$$

F 4 3 F 4 3 F

The Gaussian/GMRF-approximation



$$\pi(\boldsymbol{x} \mid \boldsymbol{y}, \boldsymbol{\theta}) \propto \exp\left(-\frac{1}{2}\boldsymbol{x}^{T}\boldsymbol{Q}\boldsymbol{x} + \sum_{i}\log\pi(y_{i}|x_{i})\right)$$
$$\approx \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{T}(\boldsymbol{Q}+\operatorname{diag}(c_{i}))(\boldsymbol{x}-\boldsymbol{\mu})\right) = \pi_{G}(\boldsymbol{x}|\boldsymbol{\theta},\boldsymbol{y})$$

Constructed as follows:

- Locate the mode **x***
- Expand to second order

Markov properties are preserved!

The Gaussian/GMRF-approximation



$$\pi(\boldsymbol{x} \mid \boldsymbol{y}, \boldsymbol{\theta}) \propto \exp\left(-\frac{1}{2}\boldsymbol{x}^{T}\boldsymbol{Q}\boldsymbol{x} + \sum_{i}\log\pi(y_{i}|x_{i})\right)$$
$$\approx \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{T}(\boldsymbol{Q}+\operatorname{diag}(c_{i}))(\boldsymbol{x}-\boldsymbol{\mu})\right) = \pi_{G}(\boldsymbol{x}|\boldsymbol{\theta},\boldsymbol{y})$$

Constructed as follows:

- Locate the mode x*
- Expand to second order

Markov properties are preserved!



Compute and approximation to the integral

$$\int \exp(ng(x)) \, dx$$

where *n* is the parameter going to ∞ .

Let x_0 be the mode of g(x) and assume $g(x_0) = 0$:

$$g(x) = \frac{1}{2}g''(x_0)(x-x_0)^2 + \cdots$$



Compute and approximation to the integral

$$\int \exp(ng(x)) \, dx$$

where *n* is the parameter going to ∞ .

Let x_0 be the mode of g(x) and assume $g(x_0) = 0$:

$$g(x) = \frac{1}{2}g''(x_0)(x-x_0)^2 + \cdots$$



Then

$$\int \exp(ng(x)) \, dx = \sqrt{\frac{2\pi}{n(-g''(x_0))}} + \cdots$$

- As $n \to \infty$, then the integrand gets more and more peaked.
- Error should tends to zero as $n \to \infty$
- Detailed analysis gives

$$\frac{\mathsf{Estimate}(n)}{\mathsf{True}} = 1 + \mathcal{O}(1/n)$$



Then

$$\int \exp(ng(x)) \ dx = \sqrt{\frac{2\pi}{n(-g''(x_0))}} + \cdots$$

- As $n \to \infty$, then the integrand gets more and more peaked.
- Error should tends to zero as $n o \infty$
- Detailed analysis gives

$$\frac{\mathsf{Estimate}(n)}{\mathsf{True}} = 1 + \mathcal{O}(1/n)$$



Then

$$\int \exp(ng(x)) \, dx = \sqrt{\frac{2\pi}{n(-g''(x_0))}} + \cdots$$

- As $n \to \infty$, then the integrand gets more and more peaked.
- Error should tends to zero as $n \to \infty$
- Detailed analysis gives

$$\frac{\mathsf{Estimate}(n)}{\mathsf{True}} = 1 + \mathcal{O}(1/n)$$



Then

$$\int \exp(ng(x)) \ dx = \sqrt{\frac{2\pi}{n(-g''(x_0))}} + \cdots$$

- As $n \to \infty$, then the integrand gets more and more peaked.
- Error should tends to zero as $n \to \infty$
- Detailed analysis gives

$$\frac{\text{Estimate}(n)}{\text{True}} = 1 + \mathcal{O}(1/n)$$

Extension I



$$g_n(x) = \frac{1}{n} \sum_{i=1}^n g_i(x)$$

then the mode x_0 depends on *n* as well.

ヨト・モラト

Extension II



$\int \exp(ng(\boldsymbol{x})) \, d\boldsymbol{x}$

and **x** is multivariate, then

$$\int \exp(ng(\mathbf{x})) \, d\mathbf{x} = \sqrt{\frac{(2\pi)^n}{n|-\mathbf{H}|}}$$

where *H* is the hessian (matrix) at the mode

$$H_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} g(\boldsymbol{x}) \Big|_{\boldsymbol{x} = \boldsymbol{x}_0}$$

(日)

Extension II



$$\int \exp(ng(\boldsymbol{x})) \, d\boldsymbol{x}$$

and **x** is multivariate, then

$$\int \exp(ng(\mathbf{x})) d\mathbf{x} = \sqrt{\frac{(2\pi)^n}{n|-\mathbf{H}|}}$$

where H is the hessian (matrix) at the mode

$$H_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} g(\boldsymbol{x}) \bigg|_{\boldsymbol{x} = \boldsymbol{x}_0}$$

<ロト < 聞 > < 国 > < 耳

Computing marginals



• Our main issue is to compute marginals

- We can use the Laplace-approximation for this issue as well
- A more "statistical" derivation might be appropriate

Computing marginals



- Our main issue is to compute marginals
- We can use the Laplace-approximation for this issue as well
- A more "statistical" derivation might be appropriate

Computing marginals



- Our main issue is to compute marginals
- We can use the Laplace-approximation for this issue as well
- A more "statistical" derivation might be appropriate

Computing marginals...



Consider the general problem

• θ is hyper-parameter with prior $\pi(\theta)$

- x is latent with density $\pi(x|\theta)$
- *y* is observed with likelihood $\pi(y|x)$

then

$$\pi(\theta|y) = \frac{\pi(x,\theta|y)}{\pi(x|\theta,y)}$$

for any x!

Computing marginals...



Consider the general problem

- θ is hyper-parameter with prior $\pi(\theta)$
- *x* is latent with density $\pi(x|\theta)$

• *y* is observed with likelihood $\pi(y|x)$

then

$$\pi(\theta|y) = \frac{\pi(x,\theta|y)}{\pi(x|\theta,y)}$$

for any x!
Computing marginals...



Consider the general problem

- θ is hyper-parameter with prior $\pi(\theta)$
- *x* is latent with density $\pi(x|\theta)$
- *y* is observed with likelihood $\pi(y|x)$

then

$$\pi(heta|y) = rac{\pi(x, heta|y)}{\pi(x| heta,y)}$$

for any x!

Computing marginals...



Some details

$$\pi(\theta|y) = \frac{\pi(x,\theta|y)}{\pi(x|\theta,y)}$$

$$\propto \frac{\pi(\theta) \ \pi(x|\theta) \ \pi(y|x)}{\pi(x|\theta,y)}$$

$$\approx \frac{\pi(\theta) \ \pi(x|\theta) \ \pi(y|x)}{\pi_G(x|\theta,y)}\Big|_{x=x^*(\theta)}$$

where $\pi_G(x|\theta, y)$ is the Gaussian approximation of $\pi(x|\theta, y)$ and $x^*(\theta)$ is the mode.

イロト イポト イヨト イヨト



Result:³

With n repeated measurements y of the same x, then

$$\frac{\widetilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y}_n)}{\pi(\boldsymbol{\theta}|\boldsymbol{y}_n)} = 1 + \mathcal{O}(n^{-3/2})$$

after renormalisation.

Relative error is a very very very nice property!

The error-rate is impressive!

Unfortunately, the assumptions made are not usually valid...

³ Tierney & Kadane,	JASA,	1986
--------------------------------	-------	------

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa



Result:³

With n repeated measurements y of the same x, then

$$\frac{\widetilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y}_n)}{\pi(\boldsymbol{\theta}|\boldsymbol{y}_n)} = 1 + \mathcal{O}(n^{-3/2})$$

after renormalisation.

Relative error is a very very very nice property!

The error-rate is impressive!

Unfortunately, the assumptions made are not usually valid...

³ Tierney & Kadane,	JASA,	1986
--------------------------------	-------	------

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa



Result:³

With n repeated measurements y of the same x, then

$$\frac{\widetilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y}_n)}{\pi(\boldsymbol{\theta}|\boldsymbol{y}_n)} = 1 + \mathcal{O}(n^{-3/2})$$

after renormalisation.

Relative error is a very very very nice property!

The error-rate is impressive!

Unfortunately, the assumptions made are not usually valid...

³ Tierney & Kadane,	JASA, 1986
--------------------------------	------------

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa



Result:³

With n repeated measurements y of the same x, then

$$\frac{\widetilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y}_n)}{\pi(\boldsymbol{\theta}|\boldsymbol{y}_n)} = 1 + \mathcal{O}(n^{-3/2})$$

after renormalisation.

Relative error is a very very very nice property!

The error-rate is impressive!

Unfortunately, the assumptions made are not usually valid...

³Tierney & Kadane, JASA, 1986

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Summary



• This are the basic ideas

The rest are just details, but there are a lot of them...

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 111 / 135

3 1 4 3

Summary



• This are the basic ideas

• The rest are just details, but there are a lot of them...

Oct 2018 111 / 135

▶ ▲ Ξ

Extensions



Model choice/selection

- High(er) number of hyperparameters

1

∃ ► ∢

Extensions



- Model choice/selection
- Automatic detection of "surprising" observations
- High(er) number of hyperparameters

≣ ► < ≣



Chose/compare various model is important but difficult

- Bayes factors (general available)
- Deviance information criterion (DIC) (hierarchical models)

▶ ∢ ⊒

Marginal likelihood



Marginal likelihood is the normalising constant for $\widetilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y})$,

$$\widetilde{\pi}(\boldsymbol{y}) = \int \frac{\pi(\boldsymbol{\theta})\pi(\boldsymbol{x}|\boldsymbol{\theta})\pi(\boldsymbol{y}|\boldsymbol{x},\boldsymbol{\theta})}{\widetilde{\pi}_{\mathsf{G}}(\boldsymbol{x}|\boldsymbol{\theta},\boldsymbol{y})} \bigg|_{\boldsymbol{x}=\boldsymbol{x}^{\star}(\boldsymbol{\theta})} d\boldsymbol{\theta}.$$
(7)

I many hierarchical GMRF models the prior is intrinsic/improper, so this is difficult to use.

Oct 2018 114 / 135

イロト イヨト イヨト

Marginal likelihood



Marginal likelihood is the normalising constant for $\tilde{\pi}(\theta|\mathbf{y})$,

$$\widetilde{\pi}(\boldsymbol{y}) = \int \frac{\pi(\boldsymbol{\theta})\pi(\boldsymbol{x}|\boldsymbol{\theta})\pi(\boldsymbol{y}|\boldsymbol{x},\boldsymbol{\theta})}{\widetilde{\pi}_{\mathsf{G}}(\boldsymbol{x}|\boldsymbol{\theta},\boldsymbol{y})} \bigg|_{\boldsymbol{x}=\boldsymbol{x}^{\star}(\boldsymbol{\theta})} d\boldsymbol{\theta}.$$
(7)

I many hierarchical GMRF models the prior is intrinsic/improper, so this is difficult to use.

< □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > <

Deviance Information Criteria



Based on the *deviance*

$$D(\boldsymbol{x}; \boldsymbol{\theta}) = -2\sum_{i} \log(y_i \mid x_i, \boldsymbol{\theta})$$

and

$$DIC = 2 \times \text{Mean} (D(\boldsymbol{x}; \boldsymbol{\theta})) - D(\text{Mean}(\boldsymbol{x}); \boldsymbol{\theta}^*)$$

This is quite easy to compute

Håvard Rue (haavard.rue@kaust.edu.sa)

▶ ∢ ⊒

Bayesian Cross-validation



Easy to compute using the INLA-approach

$$\pi(y_i \mid \boldsymbol{y}_{-i}) = \int_{\boldsymbol{\theta}} \left\{ \int_{x_i} \pi(y_i \mid x_i, \boldsymbol{\theta}) \ \pi(x_i \mid \boldsymbol{y}_{-i}, \boldsymbol{\theta}) \ dx_i \right\} \pi(\boldsymbol{\theta} \mid \boldsymbol{y}_{-i}) \ d\boldsymbol{\theta}$$

where

$$\pi(\mathbf{x}_i \mid \mathbf{y}_{-i}, \mathbf{\theta}) \propto rac{\pi(\mathbf{x}_i \mid \mathbf{y}, \mathbf{\theta})}{\pi(y_i \mid \mathbf{x}_i, \mathbf{\theta})}$$

Require a one-dimensional integral for each *i* and θ .

Oct 2018 116 / 135

3 x 4 3





Compute

$$\operatorname{Prob}(y_i^{\operatorname{new}} \leq y_i \mid \boldsymbol{y}_{-i})$$

Look for unusual large or small values

Håvard Rue (haavard.rue@kaust.edu.sa)

Part VII

Gaussian fields and GMRFs

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 118 / 135

∃ >

Gaussian fields is central in spatial statistics!

- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: O(n³)
- Difficulties: non-stationarity, space-time and curved spaces



イロト イポト イモト イモト



- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: $\mathcal{O}(n^3)$
- Difficulties: non-stationarity, space-time and curved spaces





- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: O(n³)
- Difficulties: non-stationarity, space-time and curved spaces





- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: O(n³)
- Difficulties: non-stationarity, space-time and curved spaces





- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: $\mathcal{O}(n^3)$
- Difficulties: non-stationarity, space-time and curved spaces





- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: O(n³)
- Difficulties: non-stationarity, space-time and curved spaces





- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: O(n³)
- Difficulties: non-stationarity, space-time and curved spaces





- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: *O*(*n*³)
- Difficulties: non-stationarity, space-time and curved spaces





- Covariance function, often depends only on distances
- Matérn family
- Dense covariance matrix
- Known marginal properties
- No boundary issues
- Resolution consistent
- Computational properties are not good: *O*(*n*³)
- Difficulties: non-stationarity, space-time and curved spaces







• $x_i | \mathbf{x}_{-i}$ only depends on the (few nearest) neighbours

$$\mathsf{E}(x_{ij} \mid \boldsymbol{x}_{-ij}) = \frac{1}{20} \left(8 \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{ \circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{}} \overset{\circ}{}} \overset{\circ}{\underset{\circ}{}} \overset{\circ}{}} \overset{\circ}{\underset{\circ}{}} \overset{\circ}{}} \overset{\circ}{\underset{\circ}{}} \overset{\circ}{}} \overset{\circ}{\underset{\circ}{}} \overset{\circ}{}} \overset{\circ}{} \overset{\circ}{} \overset{\circ}{} \overset{\circ}{}} \overset{\circ}{} \overset{\circ}{}} \overset{\circ}{} \overset{\circ}{} \overset{\circ}{} \overset{\circ}{}} \overset{\circ}{} \overset{\circ}{$$

- Simple conditional interpretation
- Small memory footprint
- Fast computations: $\mathcal{O}(n^{3/2})$ in \mathbb{R}^2



• $x_i | \mathbf{x}_{-i}$ only depends on the (few nearest) neighbours

$$\mathsf{E}(x_{ij} \mid \boldsymbol{x}_{-ij}) = \frac{1}{20} \left(8 \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{ \circ}} \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{\circ}} \overset{\circ}{\underset{\circ}{ \circ}} \overset{\circ}{\underset{\circ}{ \circ}{ \circ} \overset{\circ}{\underset{\circ}{ \circ}} \overset{\circ}{\underset{\circ}{ \circ}} \overset{\circ}{ \circ} \overset{\circ}{\underset{\circ}{ \circ}} \overset{\circ}{\underset{\circ}{ \circ}} \overset{\circ}{ \circ} \overset{\circ}{ } \overset{\circ}{ \circ} \overset{\circ}{ } \overset{$$

• Simple conditional interpretation

- Small memory footprint
- Fast computations: $\mathcal{O}(n^{3/2})$ in \mathbb{R}^2



• $x_i | \mathbf{x}_{-i}$ only depends on the (few nearest) neighbours

- Simple conditional interpretation
- Small memory footprint

• Fast computations: $\mathcal{O}(n^{3/2})$ in \mathbb{R}^2



• $x_i | \mathbf{x}_{-i}$ only depends on the (few nearest) neighbours

- Simple conditional interpretation
- Small memory footprint
- Fast computations: $\mathcal{O}(n^{3/2})$ in \mathbb{R}^2



Conditional modeling

- Strongest argument: Computational speed!
- Sparse matrices allow for faster computation, general algorithms
- Also relevant for sampling based inference





Conditional modeling

- Strongest argument: Computational speed!
- Sparse matrices allow for faster computation, general algorithms
- Also relevant for sampling based inference





- Strongest argument: Computational speed!
- Sparse matrices allow for faster computation, general algorithms
- Also relevant for sampling based inference





- Conditional modeling
- Strongest argument: Computational speed!
- Sparse matrices allow for faster computation, general algorithms
- Also relevant for sampling based inference





The downside...



Not easy to specify GMRFs to get "what you want"

• The link from

 $\{\pi(x_i|\mathbf{x}_{-i})\}$

to

 $Cov(x_i, x_i)$

- is "difficult" (without computing it)
- Boundary issues
- Irregular lattices are even more difficult
- Commonly used GMRF models are not resolution consistent!



The downside...



• The link from

$$\{\pi(x_i|\mathbf{x}_{-i})\}$$

to

$$Cov(x_i, x_i)$$

is "difficult" (without computing it)

- Boundary issues
- Irregular lattices are even more difficult
- Commonly used GMRF models are not resolution consistent!





Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 122 / 135
The downside...



• The link from

$$\{\pi(\mathbf{x}_i|\mathbf{x}_{-i})\}$$

to

 $Cov(x_i, x_i)$

is "difficult" (without computing it)

- Boundary issues
- Irregular lattices are even more difficult
- Commonly used GMRF models are not resolution consistent!





The downside...



- Not easy to specify GMRFs to get "what you want"
- The link from

$$\{\pi(x_i|\mathbf{x}_{-i})\}$$

to

$$Cov(x_i, x_i)$$

is "difficult" (without computing it)

- Boundary issues
- Irregular lattices are even more difficult
- Commonly used GMRF models are not resolution consistent!



The downside...



• The link from

$$\{\pi(x_i|\mathbf{x}_{-i})\}$$

to

$$Cov(x_i, x_i)$$

is "difficult" (without computing it)

- Boundary issues
- Irregular lattices are even more difficult
- Commonly used GMRF models are not resolution consistent!





Matérn fields and the reference SPDE

The solution of this SPDE (Whittle 1954/1963)

$$(\kappa^2 - \Delta)^{\alpha/2} \boldsymbol{x}(\boldsymbol{s}) = \boldsymbol{\epsilon}(\boldsymbol{s}), \qquad \alpha = \nu + \dim/2$$

is a Gaussian field with Matérn Covariance function. Δ is the Laplacian and $\epsilon(\mathbf{s})$ is spatial Gaussian white noise.

The SPDE *is* harder to work with, *but* when we know *how* then

- manifolds (easy!)
- non-stationary (easy!)
- computational properties (very good!)
- +++







Matérn fields and the reference SPDE

The solution of this SPDE (Whittle 1954/1963)

$$(\kappa^2 - \Delta)^{\alpha/2} \boldsymbol{x}(\boldsymbol{s}) = \boldsymbol{\epsilon}(\boldsymbol{s}), \qquad \alpha = \nu + \dim/2$$

is a Gaussian field with Matérn Covariance function. Δ is the Laplacian and $\epsilon(\mathbf{s})$ is spatial Gaussian white noise.

The SPDE *is* harder to work with, *but* when we know *how* then

- manifolds (easy!)
- non-stationary (easy!)
- computational properties (very good!)
- +++









Gaussian fields/ Covariance functions Gaussian Markov Random fields

・ロト ・聞 ト ・ ヨト ・ ヨト





Gaussian fields/ Covariance functions Gaussian Markov Random fields

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

・ 注 うへで Oct 2018 124 / 135

・ロト ・聞 ト ・ ヨト ・ ヨト





・ロト ・聞 ト ・ ヨト ・ ヨト





ヘロト 人間 とくほとく ほと





A numerical solution to the SPDE can be constructed as

$$x(s) = \sum_{i=1}^{n} w_i \phi_i(s)$$

for local basis/"tent" functions $\{\phi_i(s)\}$ where the weights is a local GMRF with precision matrix $Q(\cdot)$, for $\alpha = 1, 2, 3, \ldots$

We can construct **Q** from a triangulation at no cost.





A numerical solution to the SPDE can be constructed as

$$x(s) = \sum_{i=1}^{n} w_i \phi_i(s)$$

for local basis/"tent" functions $\{\phi_i(s)\}$ where the weights is a local GMRF with precision matrix $Q(\cdot)$, for $\alpha = 1, 2, 3, \ldots$



We can construct Q from a triangulation at no cost.

How to "work" with the SPDE?

Hilbert space representation/finite element method

$$\boldsymbol{x}(\boldsymbol{u}) = \sum_{k=1}^{N} \psi_k(\boldsymbol{u}) w_k$$

for basis-functions $\{\psi_k\}$ and (Gaussian) weights $\{w_k\}$





Piecewise linear representations







Piecewise linear representations







◆□▶ ◆□▶ ◆□▶ ◆□▶

(Stochastic) Weak solution



$$(\kappa^2 - \Delta)^{\alpha/2} \boldsymbol{x}(\boldsymbol{s}) = \boldsymbol{\epsilon}(\boldsymbol{s})$$

(Stochastic) Weak solution

$$\left\{\langle\phi_k,(\kappa^2-\Delta)^{\alpha/2}\boldsymbol{x}\rangle\right\}_k \stackrel{D}{=} \{\langle\phi_k,\boldsymbol{\epsilon}\rangle\}_k$$

for all test functions $\{\phi_k\}_k$.

$$\left(\langle f,g \rangle \stackrel{\text{def}}{=} \int f(\mathbf{s})g(\mathbf{s}) \ d\mathbf{s} \right)$$

Håvard Rue (haavard.rue@kaust.edu.sa)

Oct 2018 128 / 135

Results for $\alpha = 1, 2, \dots$ (I)



$$\alpha = 1: \qquad \phi_k = (\kappa^2 - \Delta)^{1/2} \psi_k$$

$$\alpha = 2: \qquad \phi_k = \psi_k$$

Define matrices C, G and K

$$\begin{split} C_{ij} &= \langle \phi_i, \phi_j \rangle \quad i \neq j \\ G_{ij} &= \langle \nabla \phi_i, \nabla \phi_j \rangle \\ \mathbf{K} &= \kappa^2 \mathbf{C} + \mathbf{G} \end{split}$$

Håvard Rue (haavard.rue@kaust.edu.sa)

▲ E → E → Q < C
 Oct 2018 129/135

御下 イヨト イヨ

Results for $\alpha = 1, 2, \dots$ (II)

The weights are Gaussian with precision matrix ${oldsymbol Q}_{lpha,\kappa}$

$$Q_{1,\kappa} = \kappa^2 \mathbf{C} + \mathbf{G}$$
$$Q_{2,\kappa} = \mathbf{K} \mathbf{C}^{-1} \mathbf{K}$$
$$\vdots$$
$$Q_{\alpha,\kappa} = \mathbf{K} \mathbf{C}^{-1} \mathbf{Q}_{\alpha-2,\kappa} \mathbf{C}^{-1} \mathbf{K}$$

Replace **C** with a appropriate diagonal matrix: This is OK

◆□▶★録▶★臣▶★臣▶ = 臣



Result



Can "solve"

$$(\kappa^2 - \Delta)^{lpha/2} \pmb{x}(\pmb{s}) = \pmb{\epsilon}(\pmb{s}), \quad lpha = 1, 2, 3, \dots, \quad lpha =
u + \mathsf{dim}/2$$

for

- any κ
- any triangulation

at no cost!!!

"solve" means: we can write down the corresponding precision matrix for the weights, and the precision matrix is (very-)sparse/a-GMRF.

(日)

Result



Can "solve"

$$(\kappa^2 - \Delta)^{lpha/2} \pmb{x}(\pmb{s}) = \pmb{\epsilon}(\pmb{s}), \quad lpha = 1, 2, 3, \dots, \quad lpha =
u + \mathsf{dim}/2$$

for

- any κ
- any triangulation

at no cost!!!

"solve" means: we can write down the corresponding precision matrix for the weights, and the precision matrix is (very-)sparse/a-GMRF.

• • = • • = •

This was just the beginning...

Pı	Preamble v				
w	What this book is and isn't ix				
1	The R-II	Integrated Nested Laplace Approximation and the NLA package	1		
	1.1	Introduction	1		
	1.2	The INLA method	1		
	1.3	A simple example	-4		
	1.4	Additional arguments and control options	14		
	1.5	Manipulating the posterior marginals	22		
	1.6	Advanced features	23		
2	Intr	oduction to spatial modeling	37		
	2.1	Introduction	37		
	2.2	The SPDE approach	46		
	2.3	A toy example	56		
	2.4	Projection of the random field	64		
	2.5	Prediction	66		
	2.6	Triangulation details and examples	73		
	2.7	Tools for mesh assessment	86		
	2.8	Non-Gaussian response: Precipitation in Paraná	87		
3	Mo	re than one likelihood	105		
	3.1	Coregionalization model	105		
	3.2	Joint modeling: Measurement error model	113		
	3.3	Copying part of or the entire linear predictor	121		
4	Poi	nt processes and preferential sampling	31		
	4.1	Introduction	131		
	4.2	Including a covariate in the log-Gaussian Cox process	140		
	4.3	Geostatistical inference under preferential sampling	143		
5	\mathbf{Spa}	tial non-stationarity	151		
	5.1	Explanatory variables in the covariance	151		
	5.2	The Barrier model	158		
	5.3	Barrier model for noise data in Albacete (Spain)	167		



イロト イヨト イヨト



This was just the beginning...



iv	Contents	
6 Risk assessment using non-standard likelihoods 6.1 Survival analysis 6.2 Models for extremes	179 	
7 Space-time models 7.1 Discrete time domain 7.2 Continuous time domain 7.3 Lowering the resolution of a spatio-temporal model 7.4 Conditional simulation: Combining two meshes	197 	
8 Space-time applications 8.1 Space-time corregionalization model 8.2 Dynamic regression example 8.3 Space-time point process: Burkitt example 8.4 Large point process: Burkitt example 8.5 Accumulated rainfall: Hurdle Gamma model	227 227 233 239 244 254	
A List of symbols and notation	267	
B Packages used in the book		
Bibliography		
Index		



イロト イポト イヨト イヨト

Oct 2018 132 / 135

Part VIII

Learn more?

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

イロト イヨト イヨト

Two recent review papers: part I and II



ANILIA Further Cick here to view the actions into finatame: • Avogate linked flownes as PPT skildes • Avogate linked references • Depker refered articles • Second Legendes

Bayesian Computing with INLA: A Review

Håvard Rue,¹ Andrea Riebler,¹ Sigrunn H. Sørbye,² Janine B. Illian,³ Daniel P. Simpson,⁴ and Finn K. Lindgren⁵

¹Department of Mathematical Sciences, Norwegian University of Science and Technology, N-7091 Trondheim, Norway, email: hrat@math.nima.no

⁷Department of Mothematics and Statistics, The Arctic University of Norway, 9037 Tromso, Norway

⁵Centre for Research into Ecological and Environmental Modelling, School of Mathematics and Statistics, University of St. Andrews, KY16 9LZ Fife, United Kingdom

⁴Department of Mathematical Sciences, University of Bath, BAZ 7AY Bath, United Kingdom ⁵School of Mathematics, The University of Edinburgh, EH9 3FD Edinburgh, United Kingdom

Annu. Rev. Stat. Appl. 2017. 4:395-421

First published online as a Review in Advance on December 23, 2016

The Annual Review of Statistics and Its Application is online at statistics annual reviews.org

This article's doi: 10.1146/annurev-statistics-060116-054045

Copyright (c) 2017 by Annual Reviews. All rights reserved

Keywords

Gaussian Markov random fields, Laplace approximations, approximate Bayesian inference, latent Gaussian models, numerical integration, sparse matrices

Abstract

The key operation in Bayesian inference is to compute high-dimensional integrals. An old approximate technique is the Laplace method or approximation, which dates back to Pierre-Simon Laplace (1774). This simple idea

イロト イポト イヨト イヨト

Two recent review papers: part I and II



AMILIAL Further Click here to view this article's online features: Download figures as PPT slides
 Navigate linked references

Bayesian Computing with INLA: A Review

Håvard Rue,1 Andrea Riebler,1 Sigrunn H. Sørbye,2 Janine B. Illian,3 Daniel P. Simpson,4 and Finn K. Lindgren5

Department of Mathematical Sciences, Norwegian University of Science and Technology, N-7991 Trondhrim Norseas: email: hmeRmath.ntm.no

⁷Department of Mathematics and Statistics, The Arctic University of Norway, 9037 Tromso,

5 Centre for Research into Ecological and Environmental Modelling, School of Mathematics and Statistics, University of St. Andrews, KY16 9LZ Fife, United Kingdom

⁴Department of Mathematical Sciences, University of Bath, BA2 7AY Bath, United Kingdom School of Mathematics. The University of Edinbursh. EH9 WD Edinbursh. United Kingdom

Annu. Rev. Stat. Appl. 2017, 4:395-421

First published online as a Review in Advance on

The Annual Review of Statistics and Its Application is online at statistics annualreviews.org

10.1146/annurev-statistics-060116-054045

Copyright (c) 2017 by Annual Reviews. All rights reserved

Keywords

Gaussian Markov random fields, Laplace approximations, approximate Bayesian inference, latent Gaussian models, numerical integration, sparse

Abstract

The key operation in Bayesian inference is to compute high-dimensional integrals. An old approximate technique is the Laplace method or approximation, which dates back to Pierre-Simon Laplace (1774). This simple idea Received: 19 February 2018 Revised: 22 May 2018 Accepted: 26 May 2018

DOI: 10.1002/wics.1445

WILEY WIRES

ADVANCED REVIEW

Spatial modeling with R-INLA: A review

Haakon Bakka1 | Håvard Rue1 | Geir-Arne Fuglstad2 | Andrea Riebler2 | David Bolin3 | Janine Illian4 | Elias Krainski5 | Daniel Simpson6 | Finn Lindgren7

CEMSE Division. King Abdullah University of Science and Technology, Thuwal, Saudi Arabia ²Department of Mathematical Sciences Norwegian University of Science and Technology,

Troubeirs Norway 3Department of Mathematical Sciences, Chalmers University of Technology and University of

Gothenhure, Gothenhure, Sweden ⁴CREEM, School of Mathematics and Statistics, University of St Andrews, St. Andrews, UK ⁵Departamento de Estatística, Universidade

Federal do Paraná, Paraná, Brazil

3School of Mathematics, University of Edinburgh,

Edinbergh, US Correspondence

Histori Rue CEMSE Division King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Coming up with Bayesian models for spatial data is easy, but performing inference with them can be challenging. Writing fast inference code for a complex spatial model with realistically-sized datasets from scratch is time-consuming, and if changes are made to the model, there is little guarantee that the code performs well. The key advantages of R-INLA are the ease with which complex models can be created and modified, without the need to write complex code, and the speed at which inference can be done even for spatial problems with hundreds of thousands of observations. R-INLA handles latent Gaussian models, where fixed effects, structured and unstructured Gaussian random effects are combined linearly in a linear predictor, and the elements of the linear predictor are observed through one or more likelihoods. The structured random effects can be both standard areal model such as the Besag and the BYM models, and geostatistical models from a subset of the Matérn Gaussian random fields. In this review, we discuss the large success of spatial modeling with R-INLA and the types of spatial models that can be fitted, we give an overview of recent developments for areal models, and we give an overview of the stochastic partial differential equation (SPDE) approach and some of the ways it can be extended beyond the assumptions of isotropy and separability. In particular, we describe how slight changes to the SPDE approach leads to straight-forward approaches for nonstationary spatial models and nonseparable space-time models.

◆□▶ ◆□▶ ◆□▶ ◆□▶ Oct 2018

134 / 135

شکرا Thank you



جامعة الملك عبدالله للعلوم والتقنية King Abdullah University of Science and Technology

Håvard Rue (haavard.rue@kaust.edu.sa)

bayescomp.kaust.edu.sa

Oct 2018 135 / 135

ハロン (雪) (ヨ) (ヨ)