Robust non-Gaussian models and how to fit them in Stan

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Plan and resources

Paper: Controlling the flexibility of non-Gaussian processes through shrinkage priors (Cabral, Bolin, and Rue 2022)

- Interpretable parameterization of the GH distribution
- Generic class of non-Gaussian models
- Stan implementation
- Controlling flexibility with shrinkage priors

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Bookdown: Fitting robust non-Gaussian models in Stan

Vignette: Fitting robust non-Gaussian models in Stan

Why go beyond Gaussian processes?

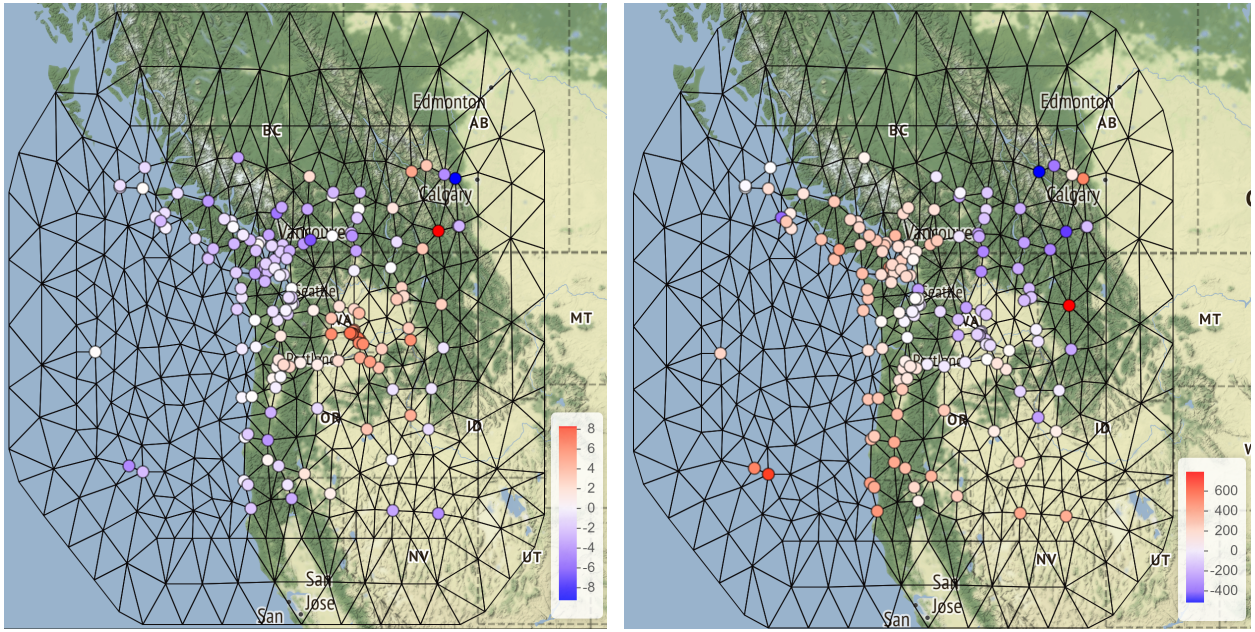

Figure 2: Measurements of temperature (left) and pressure (right)

- Gaussian processes can over-smooth in the presence of local spikes and sudden jumps in the data (Walder and Hanks 2020)
- Accommodate possible outliers in the data, and reduce their impact on the inferences (West 1984)

Why go beyond Gaussian processes?

Progression towards end stage renal failure (Asar et al. 2020)

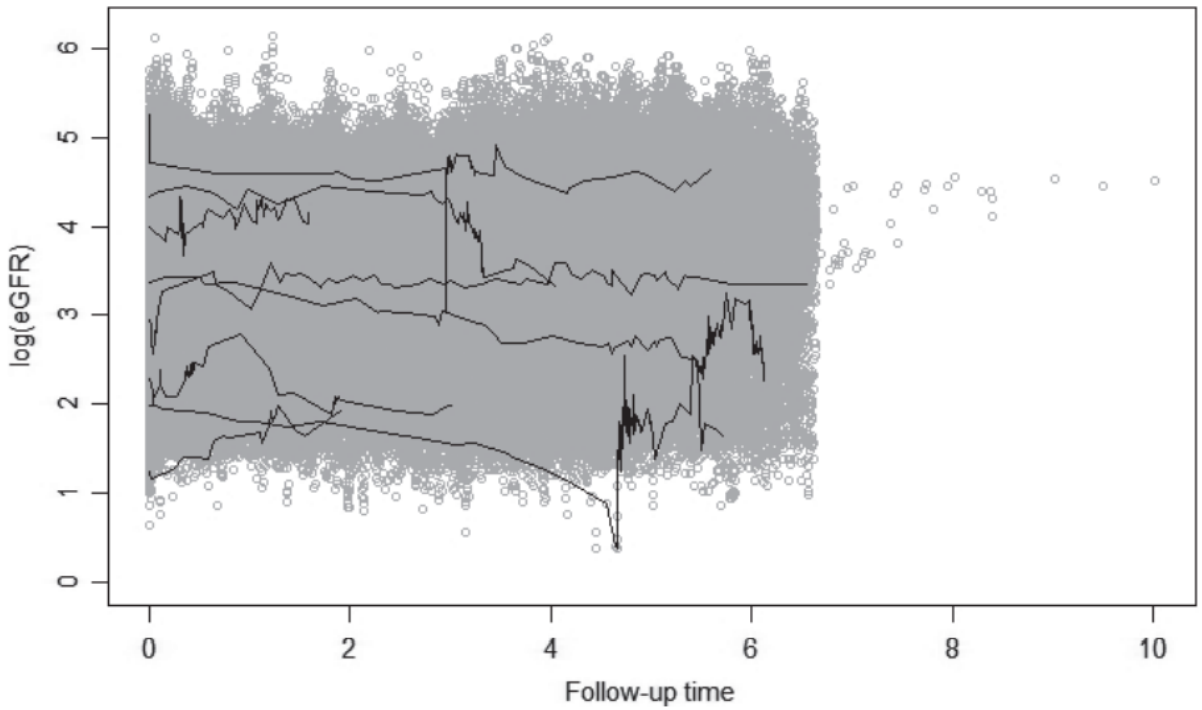

Figure 3: Log of eGFR-measurements (proxy for renal function)

What non-Gaussian models are you considering?

If $x^G \sim N(0, Q^{-1})$, with $Q = D^T D$ it can be expressed through:

$$Dx^G \stackrel{d}{=} Z,$$

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The non-Gaussian extension is:

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- Mean and covariance structure are preserved
- η and ζ control the long-tailedness and skewness.
- $\eta = \zeta = 0$ leads to the Gaussian model

What models fit into this framework?

Example: In an RW1 process we assume $x_{i+1} - x_i \sim Z_i$, so

$$D = \begin{pmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & -1 & 1 & & \\ & & & \ddots & \ddots & \\ & & & & -1 & 1 \end{pmatrix},$$

which leads to the system $Dx = Z$.

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which leads to the system $\mathrm{D}x = Z$. More examples:

- i.i.d. random effects
- Random walk and autoregressive processes
- SAR and CAR processes (Walder and Hanks 2020)
- Matérn processes (Wallin and Bolin 2015)
- ...

What sample paths do these models produce?

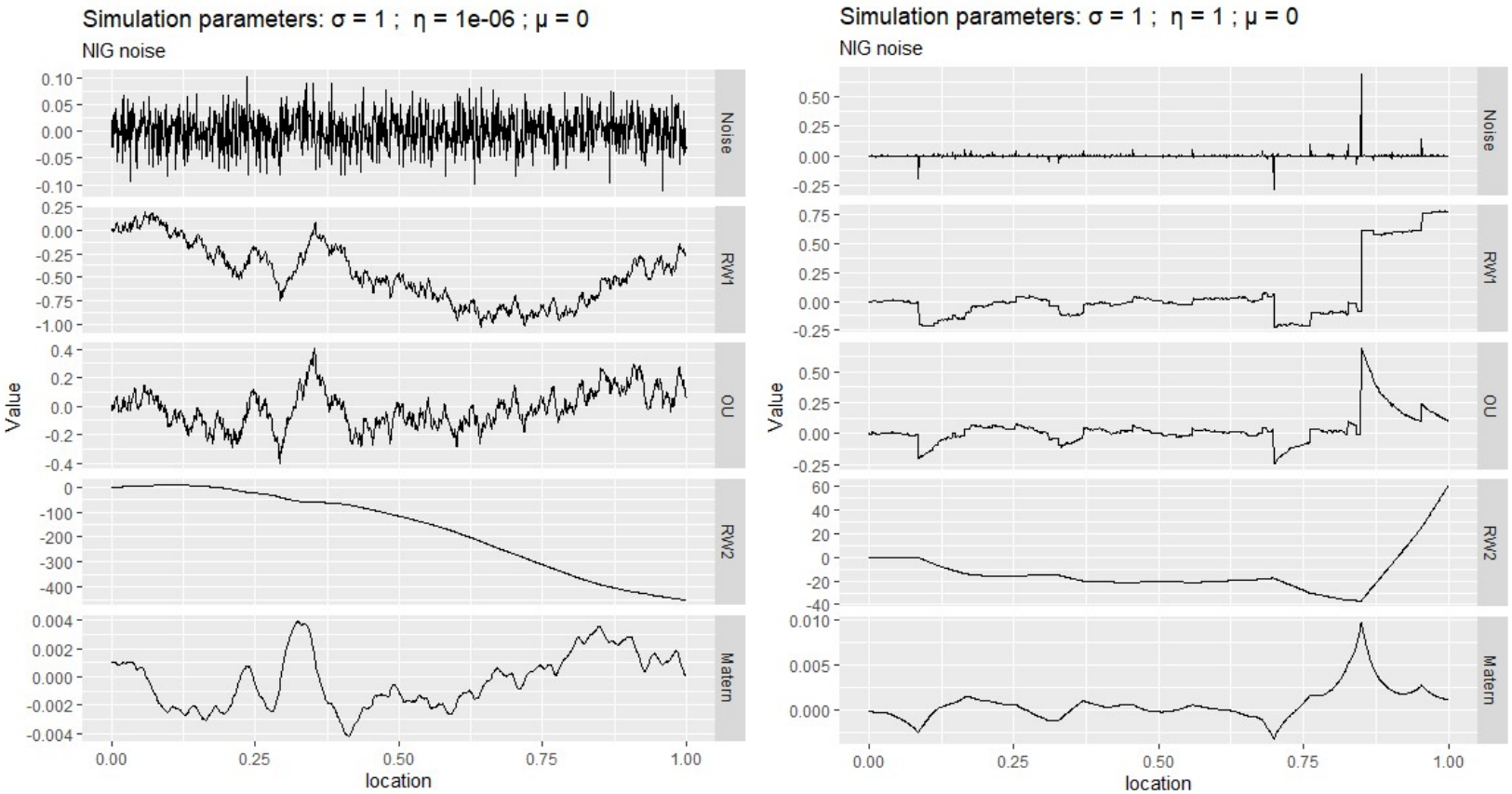

Figure 4: Sample paths of Gaussian and non-Gaussian processes.

What sample paths do these models produce?

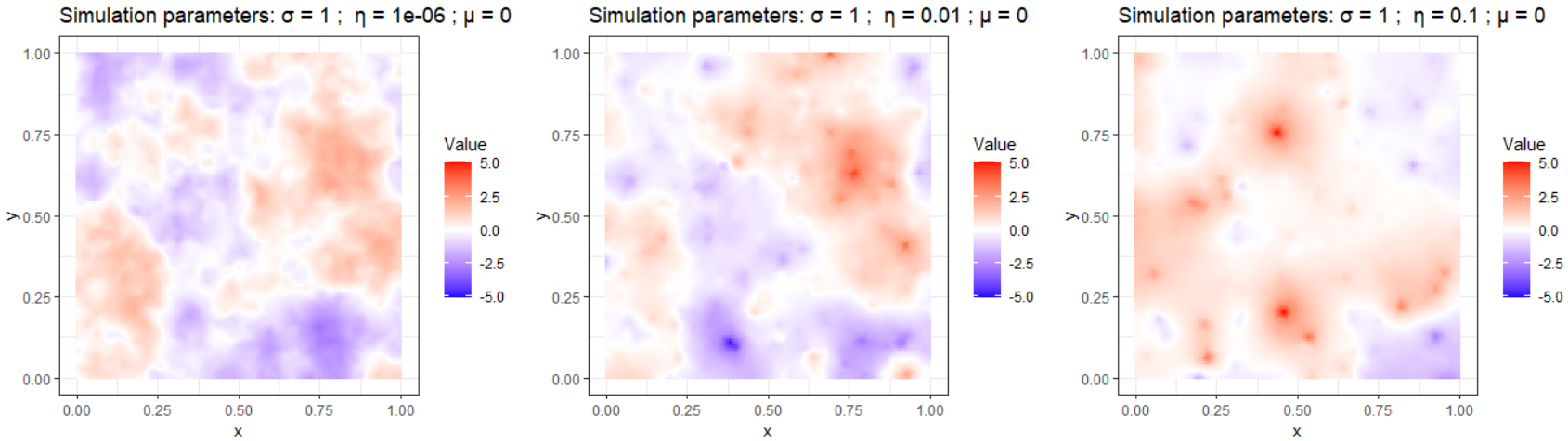

Figure 5: Sample paths of a Matérn model in 2D.

Why not just transform Gaussian processes?

- Covariates in the mean can induce a non-stationary covariance
- The mean and covariance function of the transformed process could change in non-intuitive ways (Wallin and Bolin 2015)

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With our construction, the three important model components:

- Mean
- Covariance
- Non-Gaussianity

can be modeled separately without confounding. Changing one component does not affect the others.

Stan implementation - Setup

Declaring Gaussian ($Dx = Z$) an non-Gaussian models ($Dx = \Lambda$):

```
x ~ multi_normal_prec(rep_vector(0,N), D'*D)
```

```
x ~ nig_model(D, eta, zeta, h, 1)
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Implementation performance:

- First attempt: 10 hours with poor diagnostics
- Right now: 15 minutes with very good diagnostics

Improvement 1: Collapsed representation

Other implementations relied on the normal-variance mixture:

$$\mathrm{x}|\boldsymbol{V} \sim N\left(0, \quad \mathrm{Q}^{-1}\right), \quad \mathrm{Q} = \mathrm{D}^{T}\mathrm{diag}(\boldsymbol{V})^{-1}\mathrm{D}$$

$$V_i \overset{i.i.d.}{\sim} \mathrm{IG}(1, \eta^{-1})$$

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We can, however, "integrate out" the V's:

$$\pi(\mathrm{x}) = |\mathrm{D}| \prod_{i=1}^{n} \pi_{\Lambda_i}([\mathrm{Dx}]_i),$$

- $\pi_{\Lambda_i}(x)$ is the pdf of a 1D NIG distribution
- We reduce the dimension by half
- Avoid inverting D

Improvement 2: Within-chain parallelization

$$\log \pi(x) = \log |D| + \sum_{i=1}^{n} \log \pi_{\Lambda_i}([Dx]_i),$$

```
real NIG_var_correction_lpdf(real x, real eta, real zeta, real h){
  real sigmas     = 1/sqrt(1+zeta^2*eta); //variance correction
  real hyp_alpha  = sqrt(1/eta+zeta^2)/sigmas;
  real hyp_beta   = zeta/sigmas;
  real hyp_delta  = sigmas*sqrt(1/eta)*h;
  real hyp_mu     = -sigmas*zeta*h;
  return (sqrt(hyp_alpha^2 - hyp_beta^2)*hyp_delta + hyp_beta*(x - hyp_mu) + log(hyp_alpha) +
          log(hyp_delta) - log(pi()) - 0.5*log(hyp_delta^2 + (x - hyp_mu)^2) +
          log(modified_bessel_second_kind(1, hyp_alpha*sqrt(hyp_delta^2 + (x - hyp_mu)^2))));
}
```

- $\log \pi_{\Lambda_i}$ is relatively expensive to compute
- We can evaluate $\log \pi_{\Lambda_i}([Dx]_i)$ in separate cores
- We used Stan's `reduce_sum` function

Other improvements

$$\log \pi(x) = \log |D| + \sum_{i=1}^{n} \log \pi_{\Lambda_i}([Dx]_i),$$

- Sparse matrix computations: `csr_matrix_times_vector`

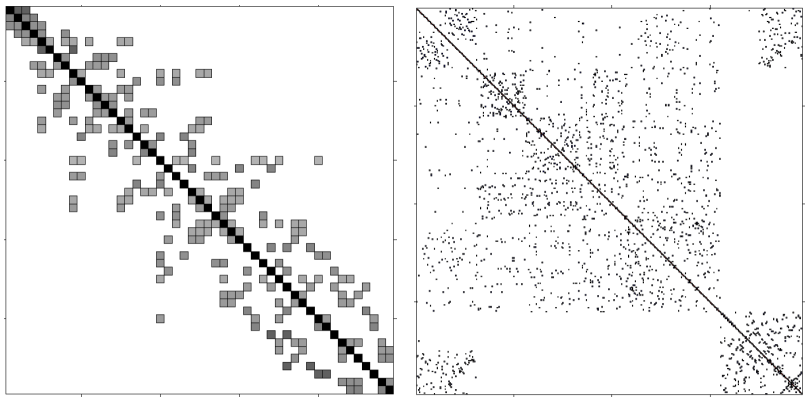
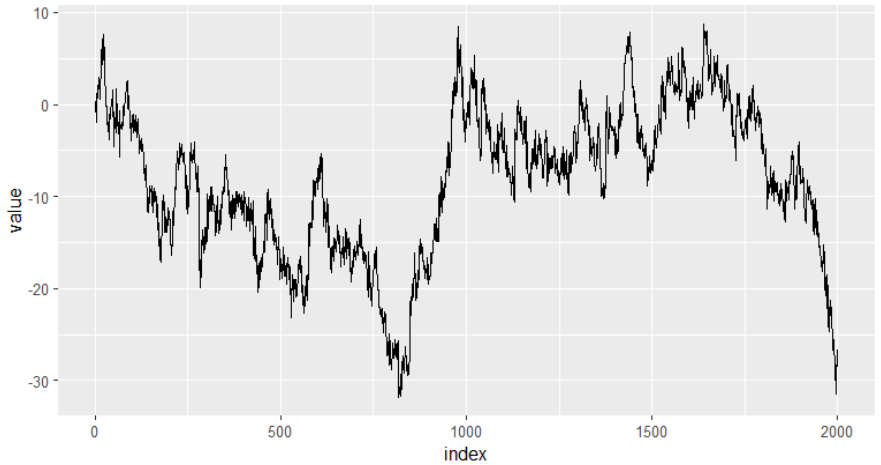


Figure 6: Matrices D for the SAR and SPDE application.

- Pre-compute your log-determinants!
  - 60% of the sampling time was spent computing determinants
  - If $D_{SAR} = I - \rho W$, then $\log |D_{SAR}| = \sum_i \log(1 - \rho v_i)$, $v_i = \text{eigen}(W)$

Simulations

Model: Hierarchical model with a latent RW1 component.



Results:

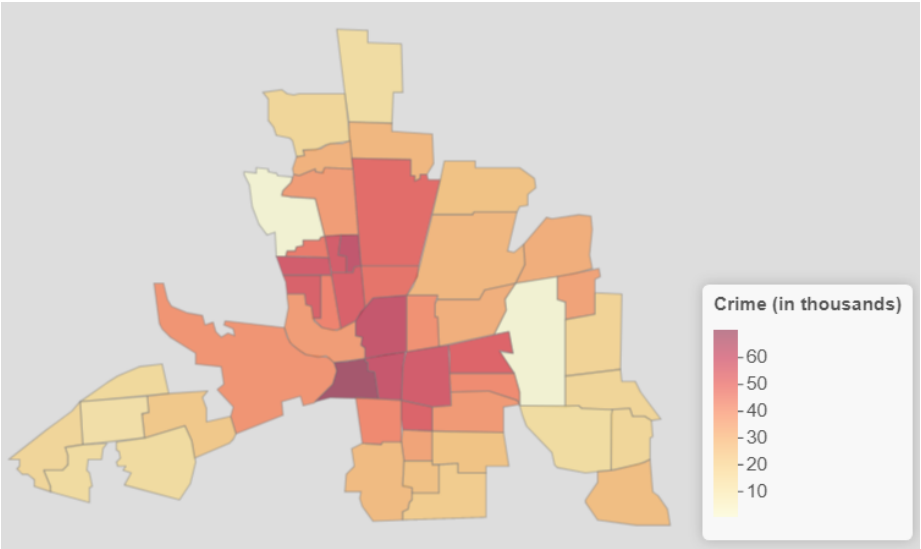
N	Implementation	ESS of η (Bulk)
2000	Variance-Mixture	0.10
	Collapsed	1.41
	Collapsed + Sparse + Parallel	5.30
4000	Variance-Mixture	0.01
	Collapsed	0.32
	Collapsed + Sparse + Parallel	2.25

Application 1: SAR model

Model:

$$y_i = \beta_0 + \beta_1 HV_i + \beta_2 HI_i + \sigma x_i,$$

- y_i: crime rates in thousands in 49 counties of Columbus, Ohio
- HV_i, HI_i: Household value and income
- x is a spatial effects SAR model ($D_{SAR} = I - \rho W$)



Application 1: SAR model

Model: $\mathsf{y} = \mathsf{B}\boldsymbol{\beta} + \sigma\mathsf{x}$

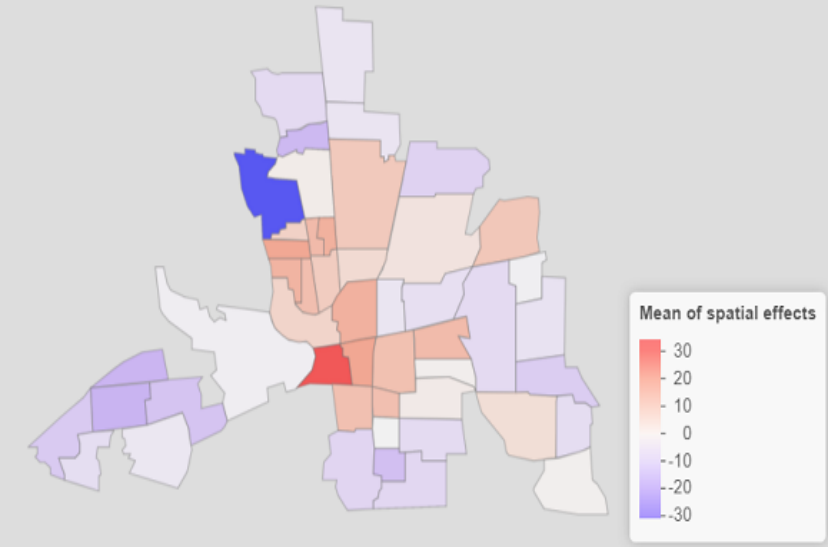
- B = design matrix
- $\mathsf{D}_{SAR}\mathsf{x} = \Lambda, \quad \mathsf{D}_{SAR} = \mathsf{I} - \rho\mathsf{W}$

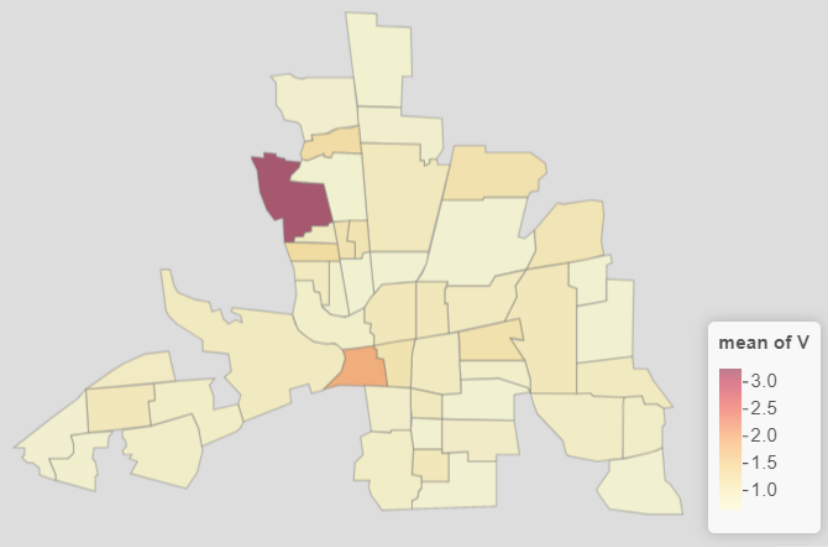
```
transformed parameters{
  vector[N] x = (y - B*beta)/sigma;      // Spatial effects
}

model{
  matrix[N,N] D = add_diag(-rho*W, 1);  // D = I - rho W
  x ~ multi_normal_prec(rep_vector(0,N), D'*D);   // Gaussian
  x ~ nig_model(D, eta, zeta, h, 1);              // NIG
  ...
}
```

Application 1: SAR model

We can identify the "outlier counties" through $E[V|y]$.





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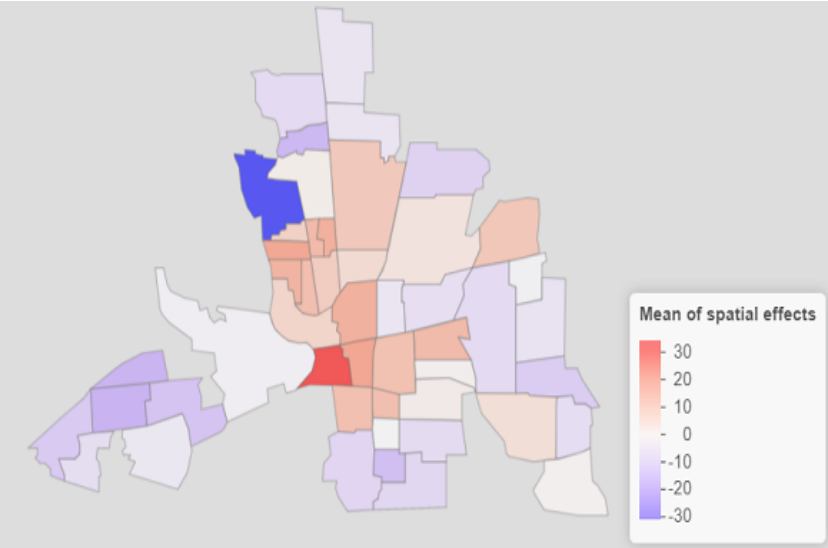

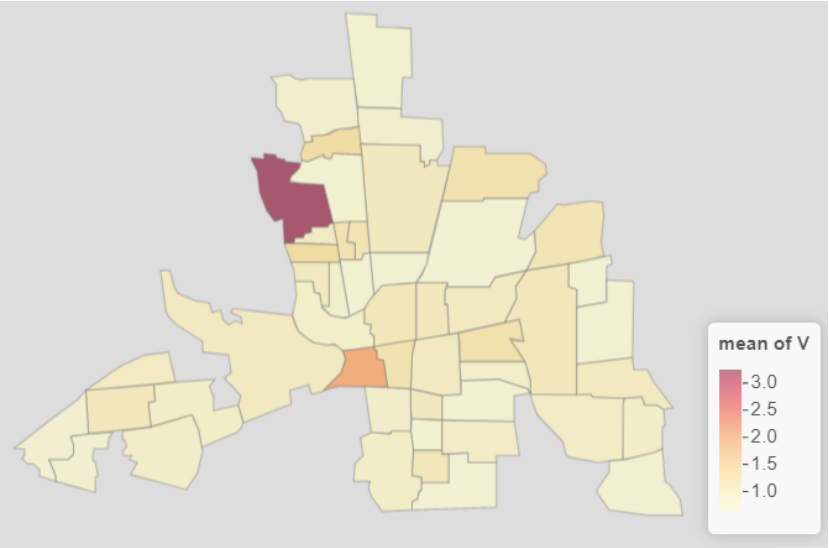

- Setup: 4 parallel chains; 2000 warmup, 3000 sampling iterations
- Gaussian model: 34s; NIG model: 93s (Collapsed only)

variable	σ	ρ	η	ζ	β_0	HV	HI
Summary	27.41	0.51	6.51	-0.11	59.30	-0.15	-1.45
q05	22.10	0.15	2.95	-1.53	33.02	-0.39	-2.38
q95	33.10	0.80	10.94	1.27	81.45	0.07	-0.50
rhat	1	1	1	1	1	1	1
ess_bulk	4578	3505	5081	1895	2091	3542	2892

Application 2: Spatial Matérn model

$X(t)$ is a Matérn Gaussian process (Whittle 1963):

$$(\kappa^2 - \Delta)^{\alpha/2} X(\mathsf{s}) = \sigma \mathcal{W}(\mathsf{s}), \quad \mathsf{s} \in \mathbb{R}^d,$$

- κ is a spatial range parameter, α is a smoothness parameter
- $\Delta = \sum_i \partial^2 / \partial x_i^2$ is the Laplace operator
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- Non-Gaussian extension: $\mathcal{W}(\mathrm{s})$ becomes $\Lambda(\mathrm{s})$
- Approximation to discrete space (Bolin 2014): $\mathrm{Dx} = \Lambda$ (FEM)

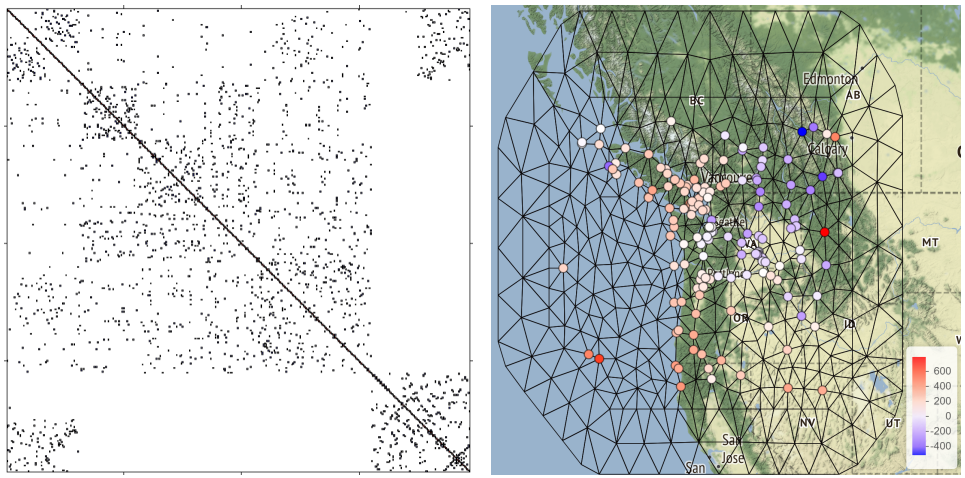

Figure 7: Matrix D (right), temperature data and mesh triangulation (right).

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Model: $y_i = x_i + \sigma_\epsilon \epsilon_i$, x is a Mátern non-Gaussian spatial field.

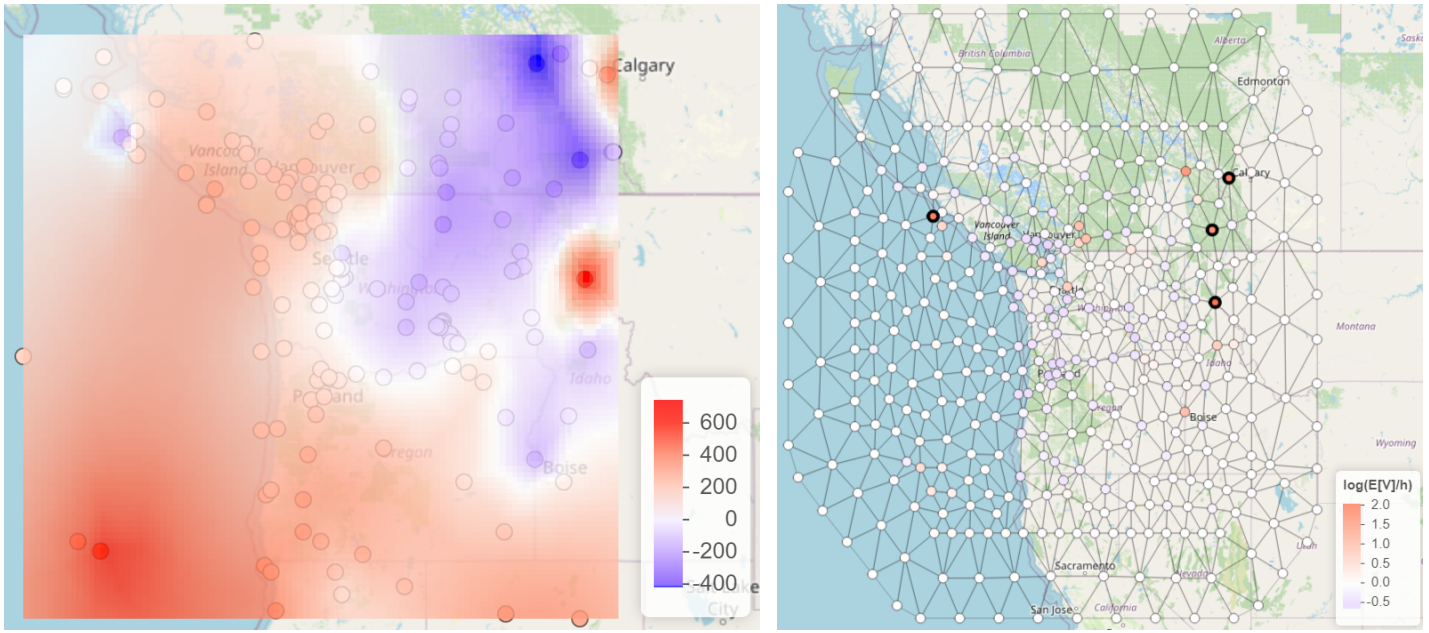

Figure 8: Posterior mean of x (left) and V (right)

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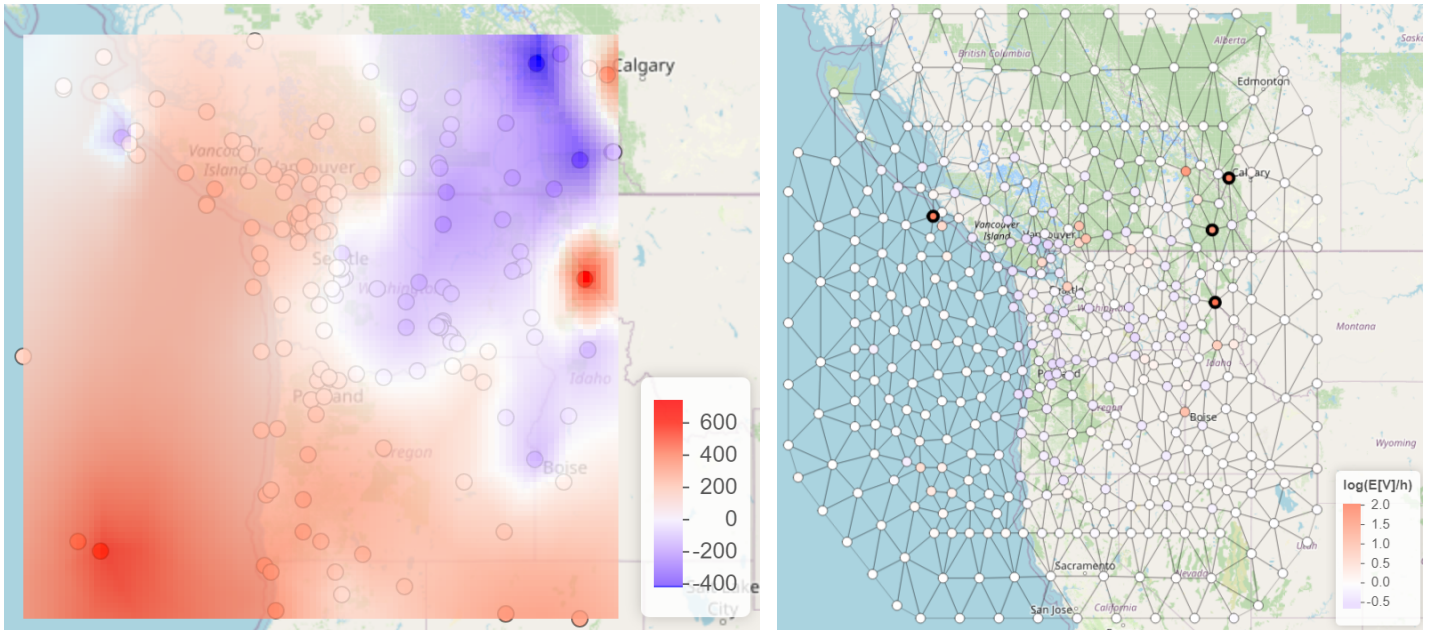

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Model	MSE	MAE	CRPS
Gaussian model	24036.848	98.647	54.893
NIG model	20246.371	87.207	53.339

Table 1: Mean squared error (MSE), mean absolute error (MAE), and continuously ranked probability score (CRPS) for the leave-one-out cross-validation predictions.

Variational Bayes in latent models

$$\mathrm{x}|\boldsymbol{V} \sim N\left(0, \quad \mathrm{Q}^{-1}\right), \quad \mathrm{Q} = \mathrm{D}^T \mathrm{diag}(\boldsymbol{V})^{-1}\mathrm{D}$$
$$V_i \overset{i.i.d.}{\sim} \mathrm{IG}(1, \eta^{-1})$$

- We find: $q(\mathrm{x}, \mathrm{V}) = q(\mathrm{x})q(\mathrm{V})$ that minimizes $\mathrm{KLD}(q(\mathrm{x}, \mathrm{V}) \mid \pi(\mathrm{x}, \mathrm{V}|\mathrm{y}))$

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  - We get an algorithm that recursively fits LGMs until convergence
  - To fit each LGM we use R-INLA (Rue et al. 2017)
- Implemented in the `ngvb` package (coming soon!).
- Example: Fitting a latent AR1 process.

```
data    <- list(x = 1:100, y = g(1:100))
formula <- y ~  f(x,  model = "ar1")
LGM     <- inla(formula, data = data)
LnGM    <- ngvb(fit = LGM, selection = list(x=1:100))
```

Berger 2013:

> *It behooves Bayesians to provide simple "standardized" Bayesian procedures with built-in robustness. While it is certainly desirable to perform specific robustness studies (...) such will require a fairly high level of sophistication. For routine use by non-experts, Bayesian procedures are needed which require minimal prior inputs and are, in some sense, inherently robust.*

Thank you for your attention!

References

Asar, Özgür et al. (2020). "Linear mixed effects models for non-Gaussian continuous repeated measurement data". In: *Journal of the Royal Statistical Society: Series C (Applied Statistics)* 69.5, pp. 1015–1065.

Berger, James O (2013). *Statistical decision theory and Bayesian analysis*. Springer Science & Business Media.

Bolin, David (2014). "Spatial Matérn fields driven by non-Gaussian noise". In: *Scandinavian Journal of Statistics* 41.3, pp. 557–579.

Cabral, Rafael, David Bolin, and Håvard Rue (2022). "Controlling the flexibility of non-Gaussian processes through shrinkage priors". In: *arXiv preprint arXiv:2203.05510*.

Rue, Håvard et al. (2017). "Bayesian computing with INLA: a review". In: *Annual Review of Statistics and Its Application* 4, pp. 395–421.

Walder, Adam and Ephraim M Hanks (2020). "Bayesian analysis of spatial generalized linear mixed models with Laplace moving average random fields". In: *Computational Statistics & Data Analysis* 144, p. 106861.

References (cont.)

Wallin, Jonas and David Bolin (2015). "Geostatistical modelling using non-Gaussian Matérn fields". In: *Scandinavian Journal of Statistics* 42.3, pp. 872–890.

West, Mike (1984). "Outlier models and prior distributions in Bayesian linear regression". In: *Journal of the Royal Statistical Society: Series B (Methodological)* 46.3, pp. 431–439.

Whittle, Peter (1963). "Stochastic processes in several dimensions". In: *Bulletin of the International Statistical Institute* 40.2, pp. 974–994.