Fast Inference for Spatial Generalized Linear Mixed Models

Based on joint work with

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Talk Summary

- Gaussian and non-Gaussian spatial data are common: disease modeling, ecology, climate science, sociology
- Spatial generalized linear mixed models (SGLMMs)
  - Popular for lattice or areal data
    Besag, York, Mollie (1991) $\approx$ 3,000 citations
  - and continuous-domain data
    Diggle et al. (1998) $\approx$ 2,000 citations
  - Very widely used in multiple disciplines
- Shortcomings of SGLMMs:
  1. Inference presents difficult computational issues, especially with large data sets
  2. Regression parameter interpretation is unreliable
- I will describe projection-based methods that simultaneously resolve both these issues

Outline

Latent Gaussian Models for Spatial Data

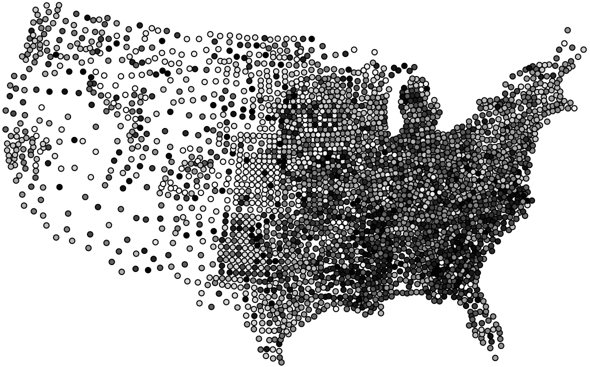
Challenges

A Solution to the Problem

Generalized Projection-based Approach

Results and Conclusions

US Infant Mortality Data by County

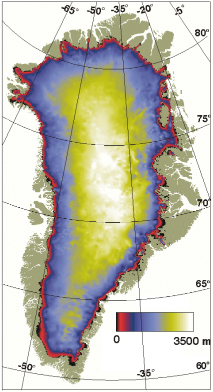


Ratio of deaths to births, each averaged over 2002-2004.

Darker indicates higher rate. $n = 3071$

Question: which factors impact infant mortality?

Greenland Ice Sheet Thickness

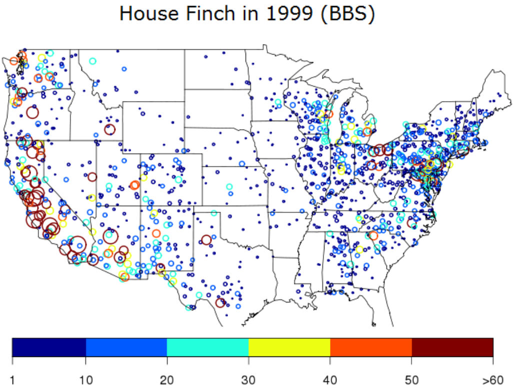


Bamber et al. (2001)

Question: How to interpolate this surface?

How to calibrate (infer parameters for) ice sheet model based on these data?

House Finch Abundances



Pardieck *et al.* 2015. *North American Breeding Bird Survey Dataset 1966 - 2014*

Question: Abundance at unsampled locations?

Models for these Data

- Spatial linear mixed models (SLMMs): for Gaussian data
- Spatial generalized linear mixed models (SGLMMs): for non-Gaussian data
- What are these models used for?
  1. interpolation (continuous-domain) or smoothing the spatial field (lattice-domain)
  2. regression while adjusting for residual spatial dependence

Spatial Linear Mixed Models (SLMMs)

- Spatial process at location $\mathbf{s} \in D \subset \mathbb{R}^d$ is

$$Z(\mathbf{s}) = X(\mathbf{s})\boldsymbol{\beta} + W(\mathbf{s})$$

  - $X(\mathbf{s})$ is covariate at $\mathbf{s}$, and $\boldsymbol{\beta}$ is a vector of coefficients
  - Model dependence among spatial random variables by imposing it on $W(\mathbf{s})$, the random effects
- Same framework works for both lattice data and continuous-domain data. Model for $W(\mathbf{s})$
  - Continuous domain: Gaussian process (GP)
  - Lattice data: Gaussian Markov Random field (GMRF)

Gaussian Processes

Infinite dimensional process $\{W(\mathbf{s}) : \mathbf{s} \in D\}$ such that

$$(W(\mathbf{s}_1), \dots W(\mathbf{s}_n))^T \mid \Theta \sim N(\mathbf{0}, \Sigma(\Theta)),$$

for $s_i \in D, \;\; i = 1, \dots, n$.

- Covariance often specified via a positive definite covariance function with parameters Θ
- E.g. (stationary) exponential covariance function
- $\Theta = (\sigma^2, \phi)$

$$\Sigma_{ij}(\Theta) = \text{Cov}(W(\mathbf{s}_i), W(\mathbf{s}_j)) = \sigma^2 \exp(-|\mathbf{s}_i - \mathbf{s}_j|/\phi)$$

Gaussian Markov Random Fields

$$(W(\mathbf{s}_1), \ldots W(\mathbf{s}_n))^T \mid \Theta \sim N(\mathbf{0}, Q(\Theta)^{-1})$$

$Q(\Theta)$ is a precision matrix based on a graph that describes a neighborhood structure: adjacencies specify dependence (skip details....)

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Inference for Spatial Linear Mixed Models

- MLE involves low-dimensional optimization

$$\arg\max_{\Theta,\beta} \mathcal{L}(\Theta, \boldsymbol{\beta}; \mathbf{Z})$$

- Bayesian inference:
  - Priors for $\Theta, \boldsymbol{\beta}$
  - Inference based on $\pi(\Theta, \boldsymbol{\beta} \mid \mathbf{Z}) \propto \mathcal{L}(\Theta, \boldsymbol{\beta}; \mathbf{Z}) p(\Theta) p(\boldsymbol{\beta})$
- Markov chain Monte Carlo with low-dimensional posterior

Literature on Computing for Spatial Linear Models

- Likelihood: high-dimensional matrices, $\mathcal{O}(n^3)$ operations
- Lots of excellent approaches that scale very well
  - Multiresolution methods, with parallelizations (Katzfuss, 2017; Katzfuss and Hammerling, 2014)
  - Nearest neighbor process (Datta et al., 2016)
  - Random projections (Banerjee, A., Tokdar, Dunson, 2013)
  - Stochastic PDEs (Lindgren et al., 2011)
  - Lattice kriging (Nychka et al., 2010)
  - Predictive process (Banerjee, Gelfand, Finley, Sang 2008)

Largely a "solved" problem

Spatial Generalized Linear Mixed Models (SGLMMs)

Model for Z at location $\mathbf{s}_i$

1. $Z(\mathbf{s}_i)|\boldsymbol{\beta}, \Theta, W(\mathbf{s}_i), i = 1, \ldots, n$, conditionally independent

   E.g. $Z(\mathbf{s}_i) \mid \boldsymbol{\beta}, W(\mathbf{s}_i) \sim$Poisson$(\mu(\mathbf{s}_i))$

2. Link function $g(\mu(\mathbf{s}_i)) = X(\mathbf{s}_i)\boldsymbol{\beta} + W(\mathbf{s}_i)$

   E.g. $\log(\mu_i) = X(\mathbf{s}_i)\boldsymbol{\beta} + W(\mathbf{s}_i)$

3. $\mathbf{W} = (W(\mathbf{s}_1), \ldots, W(\mathbf{s}_n))^T$ modeled as
   - Gaussian Markov random field model (Besag et al., 1991)
   - Gaussian processes (Diggle et al., 1998)

4. Priors for $\Theta, \boldsymbol{\beta}$

Commonly embedded within hierarchical models (cf. Banerjee, Carlin, Gelfand, 2014), say $\mathbf{Y}|\mathbf{X}$, $\mathbf{X}|\mathbf{W}$, $\mathbf{W}|\mathbf{U}, \ldots$

Challenges

Challenges posed by spatial generalized linear mixed models (SGLMMs):

(1) Computational challenges
    Rue and Held (2002, 2005), Haran (2011)

(2) Confounding between spatial random effects and fixed effects (covariates)
    Reich, Hodges, Zadnik (2006), Paciorek (2010)

Problem 1. Computational Challenge

- MLE: low-dimensional optimization of *integrated* likelihood

$$\arg\max_{\Theta,\beta} \int \mathcal{L}(\Theta, \boldsymbol{\beta}, \mathbf{W}; \mathbf{Z}) d\mathbf{W}$$

  High-dimensional integration ($\mathbf{W}$ is high-dimensional)
  MCMC-EM or MCMC-MLE: slow, challenging to implement
  (Zhang, 2002, 2003; Christensen, 2004)

- Bayesian inference based on

$$\pi(\Theta, \boldsymbol{\beta}, \mathbf{W} \mid \mathbf{Z})$$

Computing for SGLMMs

Bayes approach:

- Handle missing data easily
- Combine multiple data sets in a hierarchy
- An MCMC algorithm is easy to construct

Computing for SGLMMs

Bayes approach:

- Handle missing data easily
- Combine multiple data sets in a hierarchy
- An MCMC algorithm is easy to construct
- But... MCMC algorithms do not scale well
  - MCMC is slow per iteration due to high-dimensional

$$\pi(\Theta, \boldsymbol{\beta}, \mathbf{W} \mid \mathbf{Z})$$

  - Markov chain is slow mixing (need longer chain) due to strong cross-correlations among **W**
  - Can become impractical for large *N*

MCMC for SGLMMs

- Markov chain is slow mixing (need longer Markov chain) due to strong cross-correlations among **W**
- Block updating schemes may help. E.g. blocks:

$$\boxed{\pi(\mathbf{W} \mid \Theta, \boldsymbol{\beta}, \mathbf{Z})} \quad \boxed{\pi(\Theta \mid \boldsymbol{\beta}, \mathbf{W}, \mathbf{Z})} \quad \boxed{\pi(\boldsymbol{\beta} \mid \Theta, \mathbf{W}, \mathbf{Z})}$$

  - Challenging to obtain good proposals for **W**, especially for high-dimensions
  - Computationally expensive per update

Attempts to address these issues: Rue and Held (2005), Christensen et al. (2006), Haran and Tierney (2012)

They do not scale well (problem when $N > 1000$)

Problem 2. Spatial Confounding

- Let $P = X(X^T X)^{-1} X^T$, and $P^{\perp} = I - P$

$$g\{E(\mathbf{Z} \mid \beta, \mathbf{W}, \Theta\} = X\beta + \mathbf{W} = X\beta + \boxed{P\mathbf{W}} + P^{\perp}\mathbf{W}$$

- $P\mathbf{W}$ is in span of X
- Basic regression issue: multicollinearity

Leads to variance inflation, unstable estimates of β

(Hodges and Reich 2010; Paciorek, 2010)

Hints of the symptom, without diagnosis, by others (e.g. Diggle, 1994)

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Sketch of Our Solution

- Culprit: **W** (latent variable vector) is cause of confounding as well as computational challenges
- **W**: just a device to induce dependence
- $\boxed{\text{Idea: project } \mathbf{W} \text{ to } \delta \text{ such that}}$
  - Preserve spatial dependence implied by original **W**
  - δ is low-dimensional
  - δ is less dependent (less "cross-correlated")
  - Project orthogonal to space spanned by **X**
- Applies to both Gaussian process and GMRF models
  - GMRF models: projection based on Moran operator which uses neighborhood structure (Hughes and Haran, 2013)
  - GPs and GMRFs: general approach using eigendecomposition (Guan and Haran, 2018)

Sparse Reparameterization for GMRFs

- Regular Gaussian Markov random field $\Rightarrow$undesirable, unintended dependence structure (cf. Wall, 2004)
- Reparameterization (Hughes and Haran, 2013)
  - Deletes non-meaningful spatial dependence (weak or negative): "data-based" approach to reduce dimensions
  - Faster inference *and* a better model
- Regression coefficients are easier to interpret
- Automated MCMC is computationally efficient, allowing for routine analysis of large data sets
- Approach takes advantage of the underlying graph

What should we do in continuous-domain settings (in the absence of a graph)?

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SGLMMs with Latent Gaussian Processes

Recall: example model for count data $Z(\mathbf{s}), s \in \mathcal{D} \subset \mathbb{R}^d$.

1. Data model:

$$Z(\mathbf{s}_i) \mid \boldsymbol{\beta}, W(\mathbf{s}_i) \overset{Indep.}{\sim} \text{Poisson}(\mu(\mathbf{s}_i)), i = 1, \ldots, n$$

$$\log(\mu(\mathbf{s}_i)) = X(\mathbf{s}_i)\boldsymbol{\beta} + W(\mathbf{s}_i),$$

2. Process model: impose dependence via Gaussian process

$$\mathbf{W} \mid \sigma^2, \phi \sim N\left(\mathbf{0}, \sigma^2 \Sigma_\phi\right)$$

3. Priors for $\boldsymbol{\beta}, \sigma^2, \phi$

MCMC Inference based on posterior, $\pi(\boldsymbol{\beta}, \sigma^2, \phi, \mathbf{W} \mid \mathbf{Z})$

Posterior Distribution

$$\pi(\boldsymbol{\beta}, \sigma^2, \phi, \mathbf{W} \mid \mathbf{Z}) \propto$$

$$\prod_i^n f\left(Z(\mathbf{s}_i) \mid \beta, W(\mathbf{s}_i)\right) |\sigma^2 \Sigma_\phi|^{-\frac{1}{2}} \exp\left(-\frac{\mathbf{W}' \Sigma_\phi^{-1} \mathbf{W}}{2\sigma^2}\right) p(\boldsymbol{\beta}, \sigma^2, \phi),$$

where the covariance matrix is specified by the covariance function, for example the i, jth element

$$\Sigma_{ij} = \exp(-|\mathbf{s}_i - \mathbf{s}_j| / \phi)$$

for an exponential covariance function.

Outline of Projection-based Approach

1. Fast approximation to the principal components of Σ_ϕ
   - Approximate first m eigenvectors $U = (\mathbf{u}_1, \ldots, \mathbf{u}_m)$ and eigenvalues $D_m = \text{diag}(\lambda_1, ..., \lambda_m)$
2. Replace n-dimensional **W** with $UD_m^{1/2}\boldsymbol{\delta}$

   $\boldsymbol{\delta}$: lower dimensional and $\approx$ independent

   faster and better mixing MCMC algorithm
3. Project $UD_m^{1/2}\boldsymbol{\delta}$ to $C^\perp(X)$

   Makes random effects orthogonal to fixed effects

   handles confounding issues
4. Fit the reduced model under Bayesian framework

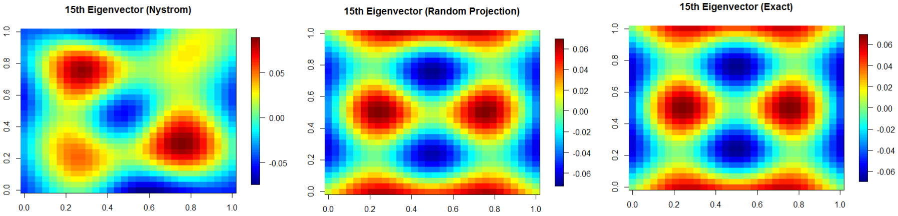
Step 1: Eigendecomposition

For speed we use a fast *approximate* eigendecomposition

Left: deterministic approximation

Center: **random approximation**

Right: exact eigendecomposition



- **Random projections** used in Banerjee, Tokdar, Dunson (2013); also Sarlos (2006), Halko et al. (2009)

Step 2: Reducing Dimensions via Projection

- Approximates the leading m eigencomponents of the covariance matrix Σ_ϕ
- **Replace W with** $UD_m^{1/2}\boldsymbol{\delta}$

Step 3: Projection to Handle Confounding

- Let $P = X(X^TX)^{-1}X^T$, and $P^\perp = I - P$
- Recall: $P\mathbf{W}$ is in span of X, causes confounding
- Solution: Remove it (cf. Reich et al., 2006; Hughes and Haran, 2013)

$$g\{E(\mathbf{Z} \mid \boldsymbol{\beta}, \mathbf{W}, \sigma^2, \phi)\} = X\boldsymbol{\beta} + \mathbf{W} = X\boldsymbol{\beta} + \cancel{P\mathbf{W}} + P^\perp\mathbf{W}$$

- High-dimensional $P^\perp\mathbf{W} \sim N(\mathbf{0}, P^\perp\Sigma P^\perp)$
  If X is nxp input matrix, then $P^\perp\Sigma P^\perp$ has rank n-p
- Only reduces dimensions from n to $n - p$
- Instead: Reduce dimension **and** confounding by $P^\perp U D_m^{1/2}\boldsymbol{\delta}$

Step 4: Inference Based on Reparameterizaion

- Spatial generalized linear mixed models

  Usual: inference based on $\pi(\boldsymbol{\beta}, \sigma^2, \phi, \mathbf{W} \mid \mathbf{Z})$
- Obtain U, D_m of Σ_ϕ
- D_m is m-dim diagonal matrix with $D_{ii} = i^{th}$ eigenvalue
- FRP: replace **W** with $UD_m^{1/2}\boldsymbol{\delta}$ to approximate SGLMM or

  RRP: replace **W** with $P^{\perp}UD_m^{1/2}\boldsymbol{\delta}$ to approximate restricted spatial model
- Reduced Model:

$$g\left\{E(Z_i \mid \boldsymbol{\beta}, U, D_m, \boldsymbol{\delta})\right\} = X_i\boldsymbol{\beta} + (P^{\perp}UD_m^{1/2})_i\boldsymbol{\delta}$$

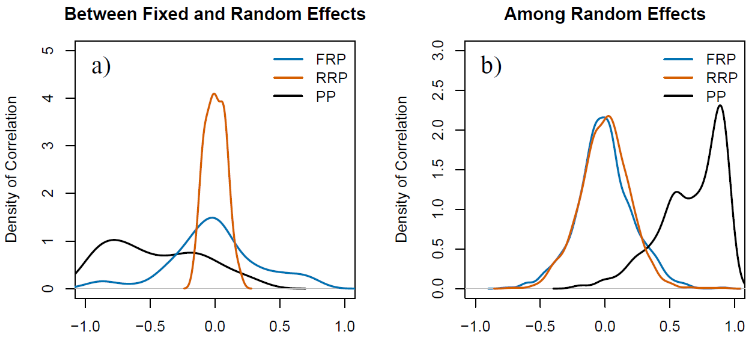
$$\boldsymbol{\delta} \mid \ldots \overset{approx}{\sim} N_m(\mathbf{0}, \sigma^2 I)$$

Now: inference based on $\pi(\boldsymbol{\beta}, \sigma^2, \phi, \boldsymbol{\delta} \mid \mathbf{Z})$

Computational Advantages: Improved MCMC Mixing

- Alleviate confounding between fixed and random effects
- Reparameterized δ are approximately independent
- De-correlating random effects: better MCMC mixing

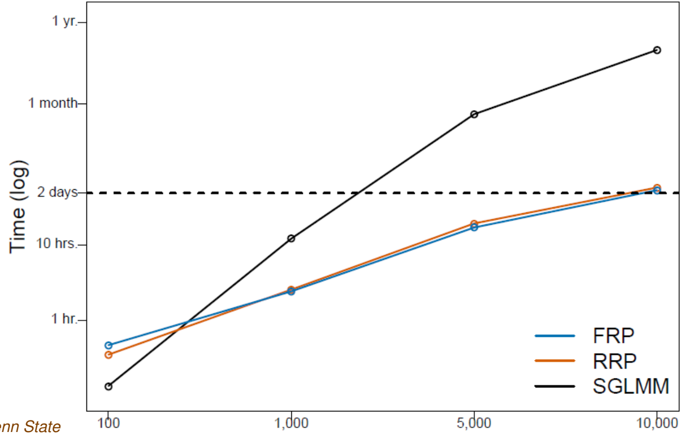
Plots of sample cross-correlations



Outline

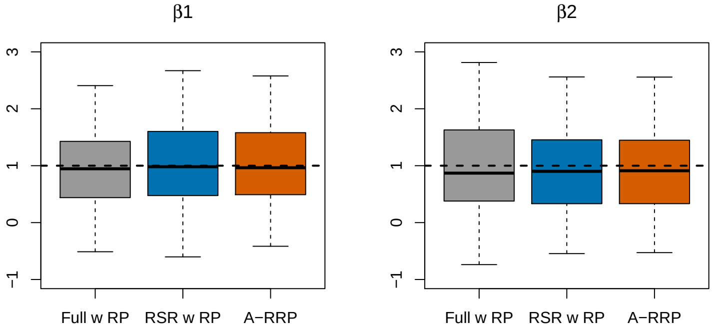
Computational Advantages: Reduced Random Effects

- Can reduce dimension of random effects, $\boldsymbol{\delta}$ to $m << n$ e.g. m = 50, n = 1000.
- Computational complexity: $O(n^2 m)$ versus $O(n^3)$ + mixing improvement (harder to quantify)



Poisson Model Simulation Study: Point Estimation

- Simulate: $\beta = (1,1)^T$, and Matérn $(\nu, \phi, \sigma^2) = (2.5, 0.2, 1)$



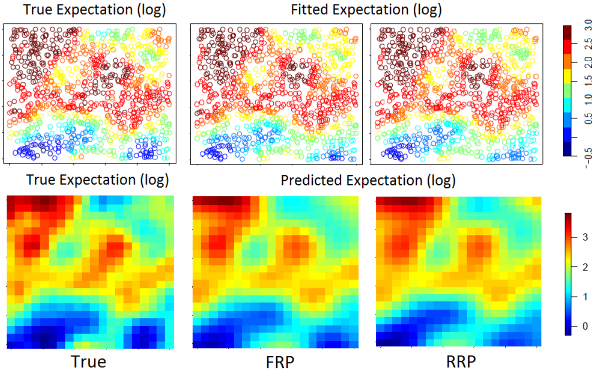
FRP: full model

RRP: restricted model (orthogonalized random effects)

A-RRP: adjusted inference

Poisson Model Prediction Performance

- Simulate n = 1000 spatial count data
- Prediction on 20 x 20 grid using rank = 50



FRP: full model

RRP: restricted model (orthogonalized random effects)

Summary

Projection-based approach

1. reduces dimensions + better MCMC mixing
2. adjusts for spatial confounding
3. simple to implement, mostly “automated”
4. good inference and prediction performance
5. other approaches (nn-GP, random-proj, Multi-Re) are better than ours for basic linear model; we are better for SGLMMs
6. extends easily to more complex hierarchical settings (not true for multiresolution-type methods even in the spatial linear model case)

Caveats and Follow-up

- Have not studied method carefully for $n > 10,000$
  - For fixed *m*, computational cost grows with *n* (mostly) due to eigendecomposition. Address via (i) discretization of space/pre-computing and (ii) other eigendecompositions
- No obvious way to adapt existing theory (e.g. pseudo-marginal MCMC) to our MCMC algorithm
- MLE: MCMC-EM algorithm with projection of latent variables at each iteration (Guan and Haran, 2018):
  - Surrogate function involves lower-dimensional integration
  - Faster than MCMC for Bayes, but trickier to construct
  - Algorithm has "probabalistic" ascent property
  - Not as easily adaptable to complicated hierarchical models

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Key References

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Frequently Asked Questions (FAQs)

- *Q. Why not use nearest neighbor Gaussian processes? (Datta et al., 2016)*
  - Works well for spatial linear mixed models
  - Effective way to reduce matrix calculations via composite likelihood. But does not reduce number of random effects
- *Q. How does your approach compare to the Gaussian predictive process (Banerjee et al., 2008)?*
  - Applicable to SGLMMs, involves dimension-reduction
  - Choice of knots can be non-trivial. Our low-dimensional representation is also “optimal”
  - Does not address spatial confounding
  - In simulated examples, we do better with prediction
  - They provide a process, we do not. But our predictions appear to be as good/better in practice

FAQs

- *Q. Is this necessary when we have the Integrated Nested Laplace Approximation (INLA) (Rue et al., 2008)?*
  - INLA is very fast
  - Hard to handle complications: (i) additional hierarchy, (ii) complicated mean structure (e.g. physical model)
  - Approximation error is fixed and hard to assess
- *Q. General relationship to fixed rank approaches?*
  - If we fixed covariance parameters, this is a fixed rank approach with fixed eigenvectors/eigenfunctions as basis
  - Eliminating small scale variations can impact SLMMs (Stein, 2014), but less impact in SGLMMs