

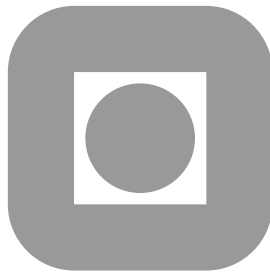
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**A note on the second order random walk model  
for irregular locations**

by

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# A note on the second order random walk model for irregular locations

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## Abstract

The second order random walk (RW2) model is commonly used for smoothing data and for modelling response functions. It is computationally efficient due to the Markov properties of the joint (intrinsic) Gaussian density. For evenly spaced locations the RW2 model is well established, whereas for irregularly spaced locations there is no well established construction in the literature. By considering the RW2 model as the solution of a stochastic differential equation (SDE), a discretely observed integrated Wiener process, it is possible to derive the density preserving the Markov properties by augmenting the state-space with the velocities. In this note, we derive a computationally more efficient RW2 model for irregular locations using a Galerkin approximation to the solution of the SDE without the need of augmenting the state-space. Numerical comparison with the exact solution demonstrates that the error in the Galerkin approximation is small and negligible in applications.

KEYWORDS: Galerkin approximation, Integrated Wiener process, Intrinsic Gaussian Markov random fields, Numerical methods for sparse matrices, Second order random walk.

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# 1 Introduction

The second order random walk (RW2) model for regular locations has the density

$$\pi(\mathbf{x}) \propto \exp\left(-\frac{1}{2} \sum_{i=3}^n (x_i - 2x_{i-1} + x_{i-2})^2\right) \quad (1)$$

where  $\mathbf{x} = [x_1, \dots, x_n]^T$ . The density is invariant under addition of  $a + bi$  to  $x_i$  for any constants  $a$  and  $b$ , and is therefore improper with rank deficiency two. The term  $x_{i+1} - 2x_i + x_{i-1}$  can be interpreted as an estimate of the second order derivative of a continuous time function  $x(t)$  at  $t = i$  using values of  $x(t)$  at  $t = i - 1$ ,  $i$ , and  $i + 1$ . Hence, the RW2 model is appropriate for representing “smooth curves” with small squared second derivative. We write “curves” to indicate that often in practice, a straight line is drawn (and is often implicit) in-between  $x_i$  and  $x_{i+1}$  as an interpolant.

The RW2 model (1) is much used in statistics, in basic tasks such as smoothing data and modelling response functions, where semi-parametric regression, smoothing and penalised likelihood are methods used (Fahrmeir and Tutz, 2001, Fahrmeir and Lang, 2001, Green and Silverman, 1994, Fahrmeir and Knorr-Held, 2000). All these tasks are important ingredients in many statistical models and are used in many areas in statistics. Rue and Held (2005, Ch. 1) gives numerous examples and references.

The popularity of (1) can be explained by two reasons. The RW2 model is quite flexible due to its invariance to addition of a linear trend, and also computationally convenient due to its Markov properties

$$\pi(x_i | \mathbf{x}_{-i}) = \pi(x_i | x_{i-2}, x_{i-1}, x_{i+1}, x_{i+2}) \quad (2)$$

for  $2 < i < n - 2$ , and with trivial changes near the boundary. Here,  $\mathbf{x}_{-i}$  denote all elements in  $\mathbf{x}$  except for  $x_i$ . The Markov property allows both for fast calculations of the related full conditionals in Markov chain Monte Carlo algorithms, but also, more efficiently, for using direct simulation algorithms based on the Kalman filter, see for example (Kitagawa and Gersch, 1996). The RW2 model is also a Gaussian Markov random field (GMRF) for which more general and very efficient simulation algorithms exist based on numerical methods for sparse matrices, see Rue and Held (2005).

Although (1) is appropriate for regular locations, we often encounter situations where  $\{x_i\}$  should represent a smooth “curve” at locations  $\{s_i\}$  where the distance between the  $s_i$ ’s are not constant. One such example, is when (1) represents the effect of a covariate in a generalised linear model and the different values of the covariate is not regularly spaced, see Rue and Held (2005, Ch. 4) for many such examples. An alternative approach in such cases, is to use regular locations and to use the value of the interpolant at  $s_i$ . This however, often leads to increased dimension of the RW2 model, which implies increased computational effort. A better approach, is to extend the RW2 model (1) to deal with irregular locations.

Let  $s_1 < s_2 < \dots < s_n$  be the set of (fixed) locations and  $x_i$  be the corresponding response at  $s_i$ , for  $i = 1, \dots, n$ . There are two approaches to construct a RW2 model for irregular locations. The first is to use a weighted version of (1) where the weights are selected by some ad-hoc argument, see Fahrmeir and Knorr-Held (2000). The second is to consider the RW2 model as a discretely observed continuous time process  $x(t)$ , where  $x(t)$  is Gaussian and is the solution of

$$\Delta x(t) = \frac{dW(t)}{dt}, \quad (3)$$

where  $\Delta = \frac{d^2}{dt^2}$  and  $W(t)$  is the standard Wiener process. Such an approach can be motivated using the connection between smoothing splines and integrated Wiener processes (Wahba, 1978), and the construction of the first order random walk for irregular locations, see for example Rue and Held (2005, Ch. 3).

The solution of (3) does not have any Markov properties, meaning that  $\pi(x_i | \mathbf{x}_{-i})$  does not simplify; the precision (the inverse covariance) matrix  $\mathbf{Q}$  is dense. Refer to Rue and Held (2005, Ch. 2) for details on this issue. The solution of (3) does however have a Markov property on an augmented space

$$\tilde{\mathbf{x}} = [x_1, x'_1, \dots, x_n, x'_n]^T \quad (4)$$

where also the derivatives (velocities) at  $\{s_i\}$  are included. For this vector with  $2n$  elements, Jones (1981) and Wecker and Ansley (1983) showed how to derive the joint density that does possess a Markov property, but the computations takes about  $9/2$  the time as for the RW2 model for regular locations; see Rue and Held (2005, Ch. 3.5) for details. This fact, in addition to increased complexity, naturally requires a RW2 model for irregular locations such that (2) holds, but where the precision matrix is such that when  $n$  increases, we converge (in some sense) to the solution of (3). In this note, we give such a formulation using a Galerkin approach (see Thomée, 1984, in essence the common *finite element* method) to solve the SDE, and demonstrate that this approximation is more than appropriate to use in applications and that the error is quite small.

The plan for the rest of this note is as follows. First, the Galerkin method is used to construct a Markov random field model approximation to the SDE (3). Second, some theoretical and practical convergence properties are discussed. Third, and finally, a simple time-series representation of the model is derived.

## 2 Construction

We seek solutions to the differential (or diffusion) equation (SDE)  $\Delta x(t) = dW(t)/dt$ . Let  $\langle f, g \rangle$  denote the inner-product  $\int f(t)g(t) dt$ . A key observation is that by the definition of *weak solutions* to the SDE, the identity

$$\langle \phi, \Delta x \rangle = \langle \phi, dW/dt \rangle \quad (5)$$

must hold, for all appropriate *test functions*  $\phi(t)$ . Now, let  $\Omega$  be the space of all possible solutions to the SDE, and let  $\{\psi_i\}_{i=1,\dots,n}$  be a set of basis functions for some subspace  $\tilde{\Omega} \subset \Omega$ . A *Galerkin approximation*  $\tilde{x}$  to the SDE is constructed as a linear combination of the basis functions,

$$\tilde{x}(t) = \sum_{i=1}^n \psi_i(t) y_i \quad (6)$$

such that the joint distribution of all scalar products  $\langle \psi_i, \Delta \tilde{x} \rangle$  equals the joint distribution of all  $\langle \psi_i, \Delta x \rangle$ . The problem is thus reduced to finding the distribution of the weights  $\mathbf{y} = [y_1, \dots, y_n]^T$ .

Let  $s_1 < s_2 < \dots < s_n$  be a sequence of discretisation points, and let  $d_i = s_{i+1} - s_i$  denote the distances between these points. We construct a Galerkin approximation for  $\tilde{\Omega}$  as the set of continuous, piecewise linear functions with derivative discontinuities at  $s_i$ . A set of basis functions  $\psi_i, i = 1, \dots, n$ , is given by

$$\psi_i(t) = \begin{cases} 0, & t < s_{i-1}, \text{ undefined for } i \leq 2, \\ \frac{t-s_{i-1}}{d_{i-1}}, & s_{i-1} \leq t < s_i, \text{ undefined for } i = 1, \\ 1 - \frac{t-s_i}{d_i}, & s_i \leq t < s_{i+1}, \text{ undefined for } i = n, \\ 0, & s_{i+1} \leq t, \text{ undefined for } i \geq n-1. \end{cases} \quad (7)$$

The second order derivatives of  $\psi_3, \dots, \psi_{n-2}$  can be expressed as

$$\Delta \psi_i(t) = \frac{1}{d_{i-1}} \delta_{s_{i-1}}(t) + \left( \frac{-1}{d_i} - \frac{1}{d_{i-1}} \right) \delta_{s_i}(t) + \frac{1}{d_i} \delta_{s_{i+1}}(t), \quad i = 3, \dots, n-2, \quad (8)$$

where  $\delta_s(t)$  is a Dirac's delta function at  $s$ . Similar expressions hold for  $\psi_1, \psi_2, \psi_{n-1}$ , and  $\psi_n$ , with the exception that there are no terms containing  $\delta_{s_{-1}}, \delta_{s_1}, \delta_{s_n}$ , or  $\delta_{s_{n+1}}$ .

Using the identity (5) for each basis function  $\psi_i$ , we obtain

$$[\langle \psi_i, \Delta x \rangle]_{i=1,\dots,n} = [\langle \psi_i, dW/dt \rangle]_{i=1,\dots,n}, \quad (9)$$

where the right-hand side has a Gaussian distribution, with expectation 0 and tridiagonal covariance matrix



which means that the model in (1) can be interpreted as an (approximate) Galerkin approximation of the SDE in (3).

### 3 Convergence

#### 3.1 Theoretical discussion

The covariance properties of the approximating GMRF converges to the continuous process as the density of the discretisation time-points increases. This can be shown in the same manner as for the corresponding random field on the sphere, see Lindgren and Rue (2004), via the following observation.

The matrix  $\mathbf{H}$  can be factorised as  $\mathbf{H} = \mathbf{A}\mathbf{W}$ , where  $\mathbf{A}$  is the diagonal matrix defined above, and where each row of  $\mathbf{W}$  contain the coefficients for calculating local approximations of the Laplacian, with exact results for quadratic polynomials. Then, the precision matrix can be written  $\mathbf{Q} = \mathbf{W}^T \mathbf{A} \mathbf{A}^{-1} \mathbf{A} \mathbf{W} = \mathbf{W}^T \mathbf{A} \mathbf{W}$ , which is the same form used in Lindgren and Rue (2004), and the elements of  $\mathbf{A}$  can be interpreted as integration weights. This form is closely related to the method of *defining* a solution to the SDE through Stratonovich integration, i.e. as the limit of a trapezoidal integration scheme (see Arnold, 1974).

#### 3.2 Convergence in practice

In order to evaluate the intrinsic stationarity and variance of the constructed intrinsic GMRF, we restrict the field to a circle, looking only at periodic realisations. The variogram  $v(u, v)$  for a process  $x(t)$  on the circle,  $0 \leq t \leq \pi$ ,  $x(0) = x(\pi)$ , is defined as the variance  $V(x(u) - x(v))$ . For stationary processes, the variogram depends only on the distance (on the circle) between  $u$  and  $v$ ,  $\tau = |u - v| \in [0, l]$ , where  $l$  is the circumference.

The theoretical variogram for the SDE restricted to the unit circle can also be calculated. The eigenvalues of the Laplacian with respect to the orthonormal basis functions  $\cos(kt)/\sqrt{\pi}$ ,  $\sin(kt)/\sqrt{\pi}$ , for  $k = 0, \dots, \infty$  is  $(\lambda_{\cos,k}, \lambda_{\sin,k}) = (-k^2, -k^2)$ , which gives the spectrum  $\lambda_k = k^{-4}$ ,  $k = 1, \dots, \infty$ , for the solutions to the SDE. Through the spectral representation of the solutions, the variogram can be calculated as

$$v(\tau) = 2 \sum_{k=1}^{\infty} \frac{1 - \cos(k\tau)}{\pi k^4} = \frac{1}{24\pi} \tau^2 (2\pi - \tau)^2, \quad 0 \leq \tau \leq 2\pi, \quad (17)$$

where the infinite series can be found in Gradshteyn and Ryzhik (1994).

The variogram for the sparse Galerkin intrinsic GMRF can be obtained for all pairs  $(s_i, s_j)$  by computing  $V_{ij} = C_{ii} + C_{jj} - 2C_{ij}$ , where  $\mathbf{C}$  is the pseudo-inverse of  $\mathbf{Q}$ . A comparison between the true variogram and the model variogram is shown in Figure 1, for  $n = 10, 20$ , and  $40$ , and for both regular and irregular spacing. With regular spacing, the variograms are practically indistinguishable already for  $n = 20$ , whereas the variogram deviation in the case of uniformly distributed discretisation points is larger, and about 3 times as many time-points are needed for the same maximal error as for regular spacing. The bulk of the error appears to be a global scaling factor, and should only have a negligible impact in practical applications.

The variogram for the complete Galerkin approximation turns out to be numerically equivalent to the true solution, as anticipated by Theorem 1; The maximal variogram deviation for  $n \leq 40$  is less than  $10^{-11}$  for regular locations and  $< 10^{-6}$  for irregular locations. Additionally, this is smaller than for the exact discretisation using an augmented state space mentioned in Section 1, which can typically have a maximal deviation of  $10^{-3}$  for irregular locations, due to numerical issues.

### 4 Time-series representation

In addition to the random field representation derived in Section 2, where the full conditionals are specified, it is sometimes convenient to have a time-series representation of the random walk model, specifying the distribution of  $y_i | y_{i-2}, y_{i-1}$ . This can be obtained by moving the future time-points,  $s_{i+1}$  and  $s_{i+2}$ , toward infinity ( $d_i \rightarrow \infty$ ), in the limit removing their influence on  $y_i$ . Evaluating the limits of the conditional mean

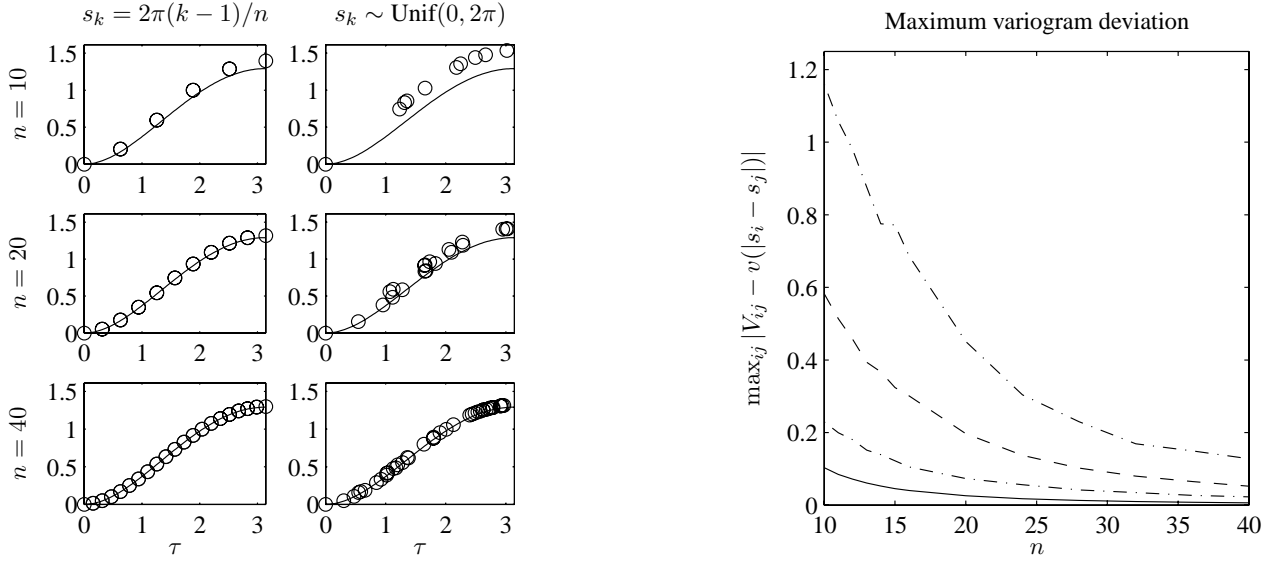


Figure 1: Left: The variogram  $V_{1,j}$  for the sparse Galerkin model (circles) compared to the exact SDE variogram (solid line) on the unit circle. Right: The maximum variogram deviation across the entire domain with regular spacing (solid line) for  $10 \leq n \leq 40$ . The mean maximum deviation for uniformly random spacing (dashed line) was estimated using 1000 replicates for each  $n$ . The dash-dotted lines show the 5%- and 95% quantiles.

and variance as  $d_i \rightarrow \infty$ , yields

$$\mathbb{E}(y_i | y_{i-1}, y_{i-2}) = \left( \frac{d_{i-1}}{d_{i-2}} + 1 \right) y_{i-1} - \frac{d_{i-1}}{d_{i-2}} y_{i-2}, \quad \mathbb{V}(y_i | y_{i-1}, y_{i-2}) = \frac{d_{i-1}^2 (d_{i-2} + d_{i-1})}{2}. \quad (18)$$

The conditional expectation is the same as given by Fahrmeir and Knorr-Held (2000), but the variance is different.

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## Appendix: Proof of Theorem 1

Let  $\Sigma$  be the covariance of the SDE sampled at  $s_1, \dots, s_n$  with circular topology of length  $l$ , conditionally on  $\int_0^l x(t) dt = 0$ . From the spectral representation of the SDE,  $\Sigma_{ij} = l^3/720 - \tau_{ij}^2(l - \tau_{ij})^2/(24l)$ , where  $\tau_{ij} = (s_j - s_i) \bmod l$ . Using the intrinsic property of the SDE, the covariance conditionally on  $\sum_{i=1}^n x(s_i) = 0$  is given by  $\tilde{\Sigma} = J\Sigma J$ , where  $J = I - \mathbf{1}\mathbf{1}^T/n$ . Recall that  $Q = H^T B^{-1} H$ .

First, we need to show that  $Q\tilde{\Sigma}Q = Q$ . For any circular topology,  $H$  and  $B$  are symmetric circulant matrices, and direct calculation shows that

$$-24l [\Sigma H]_{ij} = \begin{cases} d_{j-1}(l - d_{j-1})^2 + d_j(l - d_j)^2, & i = j, \\ d_{j-1}((2\tau_{ij} - l - d_j)^2 - 2\tau_{ij}(l - \tau_{ij})) \\ \quad + d_j((2\tau_{ij} - l + d_j)^2 - 2\tau_{ij}(l - \tau_{ij})), & i \neq j. \end{cases} \quad (19)$$

and  $H\Sigma H = B - dd^T/l$ , where  $d = B\mathbf{1}$ , so that

$$Q\tilde{\Sigma}Q = QJ\Sigma JQ = Q\Sigma Q \quad (20)$$

$$= HB^{-1}(B - dd^T/l)B^{-1}H = HB^{-1}H - H\mathbf{1}\mathbf{1}^T H/l \quad (21)$$

$$= HB^{-1}H = Q, \quad (22)$$

where we use that  $\mathbf{1}$  is an eigenvector of both  $H$  and  $Q$ , with eigenvalue 0.

The second part is more difficult. We need to show that  $\tilde{\Sigma}Q\tilde{\Sigma} = \tilde{\Sigma}$ . Expanding and simplifying the left- and right-hand sides yields  $J\Sigma HB^{-1}H\Sigma J = J\Sigma J$ . Define  $\tilde{F} = [\tau_{ij}(l - \tau_{ij})/(2l)]_{i,j=1,\dots,n}$  and  $F = \mathbf{1}a + \tilde{F}$ , for some row vector  $a$ . We will verify that  $F = \Sigma HB^{-1}$  by comparing  $\Sigma H$ , calculated above, to  $FB$ . The reader may not want to verify by direct calculation that  $[\Sigma H - \tilde{F}B]_{ij} = \mathbf{1}b$ , where  $b_j = (d_{j-1}(l^2 - d_{j-1}^2) + d_j(l^2 - d_j^2)) / (-24l)$ . Thus,  $\Sigma H = FB$  is fulfilled for  $a = bB^{-1}$ .

Finally, direct calculation of  $\tilde{F}H$  yields  $\tilde{F}H = I - \mathbf{1}d^T/l$ , so that

$$JFH = J(\mathbf{1}a + \tilde{F})H = J\tilde{F}H = J(I - \mathbf{1}d^T/l) = J \quad (23)$$

and we are done.