Supplementary Material

Use of ordinary kriging and Gaussian conditional simulation to interpolate airborne fire radiative energy density estimates

C. Klauberg^A, A. T. Hudak^{A,E}, B. C. Bright^A, L. Boschetti^B, M. B. Dickinson^C, R. L. Kremens^D and C. A. Silva^B

^AUSDA Forest Service Rocky Mountain Station, Forestry Sciences Laboratory, 1221 South Main Street, Moscow, ID 83843, USA.

^BUniversity of Idaho, 708 South Deakin Street, Moscow, ID 83844, USA.

^CUSDA Forest Service, Northern Research Station, 359 Main Road, Delaware, OH 43015, USA.

^DRochester Institute of Technology, Center of Imaging Science, 54 Lomb Memorial Drive, Rochester, NY 14623, USA.

^ECorresponding author. Email: ahudak@fs.fed.us

Background

Data transformation

High values increase the variance of the dataset and make the task of semivariogram calculation and kriging estimation more difficult (Yamamoto 2005, 2007, 2010) such that low values are overestimated, and high values underestimated (Yamamoto 2007). The solution for this type of distribution is to transform the data to obtain a symmetrical distribution.

The lognormal distribution was not simply assumed but tested based on functions for distribution fitting using the 'fitdistrplus' library package in the R programming (R Core Team 2015). We used Cullen and Frey graph analysis and AIC values to determine that the fit of the lognormal distribution was better (lower AIC) than Weibull or Gamma distributions. Estimated FRED also closely matches a power law distribution, which has the advantage of being scale invariant but can have infinite mean and variance (Mitzenmacher 2004); for some combinations of the parameters, the integration of a power law distribution with the method proposed by Kumar *et al.* (2011) returns invalid results. For these reasons, we ultimately chose to fit empirically derived estimates of FRED with a lognormal distribution.

Lognormal kriging was proposed for the first time by Journel (1980), who proposed a back-transform equation based on the kriging variance and the natural logarithm transform applied to the original data.

However, the main problem with lognormal kriging appears upon back-transformation, which introduces a bias compared with the original data (Journel and Huijbregts 1978). Several papers have reported this bias in the back-transformed estimates (Saito and Goovaerts 2000; Yamamoto 2005, 2007). Some authors have proposed an approach to transformation and back transformation of lognormal data, such as Yamamoto (2010) (Eqns S1*a*, S1*b*) and Papritz and Schwierz (2016) (Eqns S2*a*, S2*b*).

$$Y_{(x)} = log(Z_{(x)} / median_{Z(x)}) \text{ (S1a)}$$

$$Z_{back transf} (x) = Exp(Y_{OK} (x) + Y_{NSo} (x)) \times median_{Z(x)} \text{ (S1b)}$$

$$Y_{(x)} = log(Z_{(x)}) \text{ (S2a)}$$

$$Z_{back transf} (x) = Exp(Y_{OK} (x) + 0.5 \times (variance_{Y(x)} - variance_{Y_{OK}(x)})) \text{ (S2b)}$$

where: $Y_{(x)}$ = original data transformed; $Z_{(x)}$ = observed data; $Z_{back transf}(x)$ = back-transformed lognormal kriged data; $Y_{OK}(x)$ = predicted value by OK; $Y_{NSo}(x)$ is the smoothing parameter that is negative when overestimation occurs and positive otherwise.

Ordinary kriging

Kriging is a geostatistical method that takes into consideration the distance and the degree of variation between known data points, and is the best linear unbiased predictor (Journel and Huijbregts 1978; Yamamoto and Landim 2013). Kriging is a way to interpolate sample data (observations) to estimate or predict values at unsampled sites, based only on a linear model of regionalization. The linear model of regionalization is essentially a weighting function required to krig and can be graphically represented by a semivariogram. Kriging predicts the response by using the spatial correlation among the sampling points, called semivariances (e.g. Journel and Huijbregts 1978; Isaaks and Srivastava 1989; Cressie 1993). The semivariances of the points are a function of the distance between samples, known as lag distance h, according to (Eqn S3):

$$\hat{\gamma}(h) = \frac{1}{2n} \sum_{i=1}^{n} \left[z(x_i) - z(x_i + h) \right]^2$$
(S3)

where *n* is the number of local data pairs of sample points *z* separated by distance *h*, and $\hat{\gamma}(h)$ is the semivariance as a function of distance h. The semivariogram is the $\hat{\gamma}(h)$ plotted against h (Goovaerts 1997).

Semivariance typically increases with increasing distance h, which reflects decreasing autocorrelation with increasing h. Semivariograms have three main parameters, namely: 'nugget' (C_0) is the semivariance at h = 0; it is the inherent spatial variability of the process independent of the sampling frequency. The 'sill' (C_1) is the semivariance where there is no spatial correlation. The 'range' (a) is the lag distance where the semivariogram reaches the sill. Sample semivariograms describe the spatial autocorrelation for the sample dataset. Semivariogram models are made by creating a mathematical function to simulate the nugget, sill, and range, and thus the shape of the sample semivariogram. Common functions used in a semivariogram model include: linear, spherical, exponential, and Gaussian.

Ordinary kriging (OK) assigns to unsampled locations the mean calculated from local samples based on the semivariogram weighting function. It is the most widely used kriging method for its simplicity and the results it provides. OK is a location estimate method, and thus, the estimate at an unsampled point is a linear combination of the values found in a close neighbourhood (Yamamoto and Landim 2013). The OK estimator minimizes the error variance and is not biased where the average error is equal to zero.

The OK estimator is (Eqn S4):

$$\hat{z}_{OK}(x_0) = \sum_{i=1}^n \delta_i z(x_i)$$
 (S4)

where the kriging weights δ_i are determined by minimising the variance (Eqn S5):

$$var\left[\hat{z}_{OK}\left(x_{0}\right)\right] = E\left[\left\{\hat{z}\left(x_{0}\right) - z\left(x_{0}\right)\right\}^{2}\right]$$
(S5)

where $z(x_0)$ is the true value expected at point x_0 .

Experimental semivariograms that are similar in all directions reveal isotropy, whereas semivariograms with a directional component reveal anisotropy.

Although kriging pursues an estimate that represents as accurately as possible the true value of a variable at a given point, the spatial variability of the sampled values is not reproduced. In this interpolation method, the unbiased estimation is prioritized, as well as the minimization of the estimation variability (Andriotti 2004). Also, this method has some disadvantages such as bias due to some underestimation and overestimation; production of only one value for every location in the study area; and generation of interpolated surfaces that are usually smoothed images (less variable) unlike the real phenomenon (Diggle and Ribeiro 2007; Yamamoto and Landim 2013).

Gaussian conditional simulation

Due to some disadvantages of kriging, conditional simulation (CS), another geostatistical method, is a good alternative for interpolating FRED data. The spatial characteristics found in the sample data are maintained and replicated in each of n surfaces generated by the simulation method. For a given unsampled location, none of the n simulated values are the best estimator of the true but unknown value (as with OK); rather, they vary around the best estimate as defined by the dispersion of the sample data (Andriotti 2004). Hence, each unsampled location in the study area will have a distribution of values provided by the simulated surfaces (Yamamoto and Landim 2013). The spatial variability of the surfaces depends on the geostatistical properties (distribution, semivariogram, etc.) of the sample data, which are estimated before generating the conditional simulation (Renard *et al.* 2011).

For the simulations to be conditional, they must honour the measured values at sampled sites. So, functions (or surfaces) are simulated that satisfy two conditions: first, covariance (or semivariogram) of the original data is maintained and second, it passes through the points sampled (Andriotti 2004; Yamamoto and Landim, 2013). Therefore, the decomposition of the conditional simulation becomes (Andriotti 2004) (Eqn S6),

$$z(x) = z'(x) + \left[z(x) - z'(x)\right]$$
(S6)

where: z(x) = real value; z'(x) = estimated value for kriging; [z(x) - z'(x)] = error.

In this case, the error [z(x) - z'(x)] is unknown, since the real value z(x) is not available. When we simulate a realisation of a random function S(x) with the same covariance as Z(x), and where s(x) is a conditioned simulation that keeps the same pattern of available data, we have (Eqn S7):

$$s(x) = s'(x) + \left[s(x) - s'(x)\right]$$
(S7)

where: [s(x) - s'(x)] = known error.

In the first equation (Eqn 6), we replace the measured error in s(x) and define a function zs(x) (Eqn S8).

$$zs(x) = z'(x) + \left[s(x) - s'(x)\right]$$
(S8)

The function zs(x) is called conditional simulation (Eqn S8).

References

Andriotti JLS (Ed.) (2004) 'Fundamentos de estatística e geoestatística.' (Editora Unisinos: São Leopoldo, Brazil)

Cressie N (Ed.) (1993) 'Statistic for spatial data.' (Wiley: New York)

- Diggle PJ, Ribeiro PJ Jr (2007) 'Model-based geostatistics.' (Springer: New York)
- Goovaerts P (1997) 'Geostatistics for natural resources evaluation.' (Oxford University Press: New York)
- Isaaks EH, Srivastava RM (Eds) (1989) 'Applied geostatistics.' (Oxford University Press: New York)
- Journel AG (1980) The lognormal approach to predicting local distributions of selective mining unit grades. *Mathematical Geology* **12**, 285–303. doi:10.1007/BF01029417
- Journel AG, Huijbregts CJ (1978) 'Mining geostatistics.' (Academic Press: London)
- Kumar SS, Roy DP, Boschetti L, Kremens R (2011) Exploiting the power law distribution properties of satellite fire radiative power retrievals: a method to estimate fire radiative energy and biomass burned from sparse satellite observations. *Journal of Geophysical Research* **116**, D19303. doi:10.1029/2011JD015676
- Mitzenmacher M (2004) A brief history of generative models for power law and lognormal distributions. *Internet Mathematics* **1**, 226–251. doi:10.1080/15427951.2004.10129088
- Papritz A, Schwierz C (2016) Package 'georob': robust geostatistical analysis of spatial data. Available at https://cran.r-project.org/web/packages/georob/georob.pdf [Verified 20 February 2016]
- R Core Team (2015) 'R: A language and environment for statistical computing.' (R Foundation for Statistical Computing: Vienna) Available at http://www.R-project.org/ [Verified 6 May 2017]
- Renard P, Straubhaar J, Caers J, Mariethoz G (2011) Conditioning facies simulations with connectivity data. *Mathematical Geosciences* **43**, 879–903. doi:10.1007/s11004-011-9363-4
- Saito H, Goovaerts P (2000) Geostatistical interpolation of positively skewed and censored data in a dioxincontaminated site. *Environmental Science & Technology* **34**, 4228–4235. doi:10.1021/es991450y

- Yamamoto JK (2005) Correcting the smoothing effect of ordinary kriging estimates. *Mathematical Geology* **37**, 69–94. doi:10.1007/s11004-005-8748-7
- Yamamoto JK (2007) On unbiased back-transform of lognormal kriging estimates. *Computers & Geosciences* **11**, 219–234. doi:10.1007/s10596-007-9046-x
- Yamamoto JK (2010) Back-transforming rank order kriging estimates. Geologia-USP. Série Científica 10, 101– 115.
- Yamamoto JK, Landim PMB (Eds) (2013) 'Geoestatística: conceitos + aplicações.' (Oficina de Texto: São Paulo, Brazil)

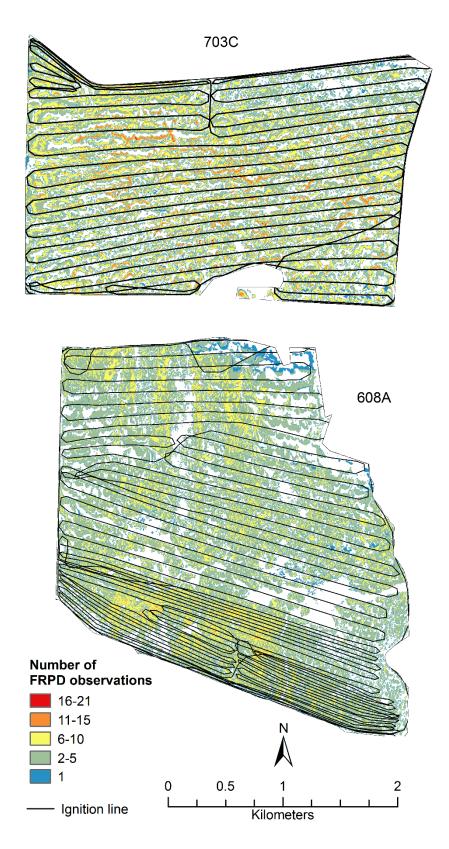


Fig. S1. Number of FRPD observations recorded by the airborne Wildland Airborne Sensor Program (WASP) instrument per active fire pixel while imaging the 2011 burn blocks. Overlaid are the helicopter ignition lines (Hudak *et al.* 2017).

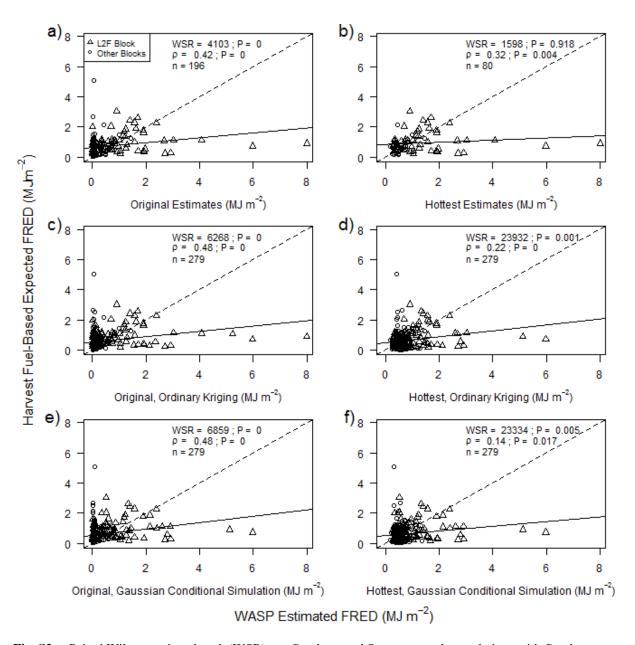


Fig. S2. Paired Wilcoxon signed-rank (WSR) test *P*-values, and Spearman rank correlations with *P*-values, comparing WASP-derived FRED estimates (*x*-axes) with expected FRED based on observations of prefire fuel load at clip plot locations, % consumption, and % water content (Table 1), as per Smith *et al.* (2013). Sample sizes of original estimates and hottest estimates are lower than from the interpolated grids because of ground-based measurement locations occurring within WASP-derived FRED data voids. Solid lines indicate the best linear fit and dotted lines the 1:1 relationship.

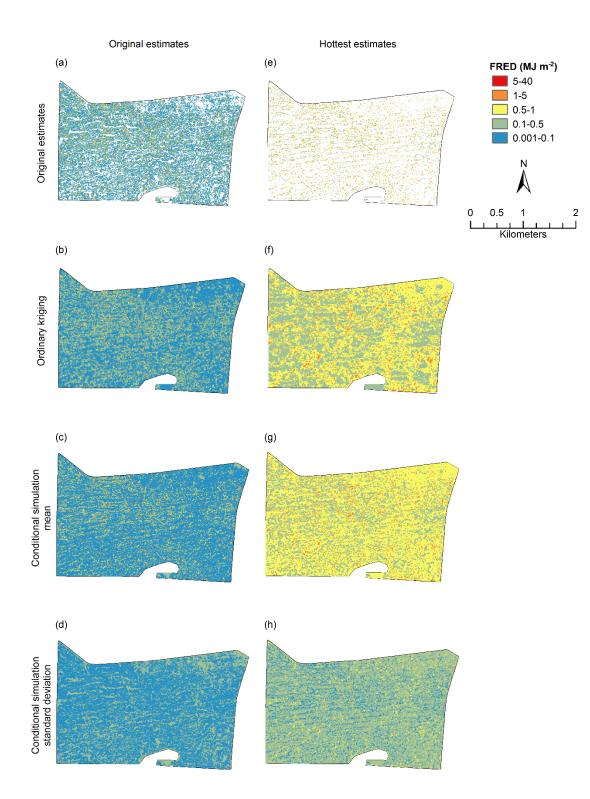


Fig. S3. Original uninterpolated (a, e), ordinary kriging (OK) interpolated (b, f), and Gaussian conditional simulation (GCS) interpolated (c, d, g, h) fire radiative energy density (FRED) maps of 2011 burn block 703C. Maps based on original FRED estimates are shown in the left column (a, b, c, d); maps based on hottest FRED estimates are shown in the right column (e, f, g, h).

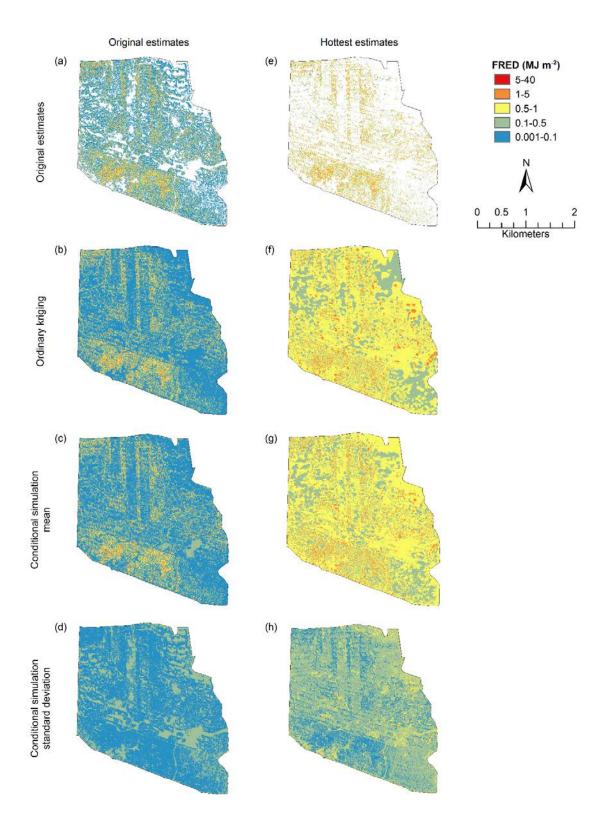


Fig. S4. Original uninterpolated (a, e), ordinary kriging (OK) interpolated (b, f), and Gaussian conditional simulation (GCS) interpolated (c, d, g, h) fire radiative energy density (FRED) maps of 2011 burn block 608A. Maps based on original FRED estimates are shown in the left column (a, b, c, d); maps based on hottest FRED estimates are shown in the right column (e, f, g, h).