

**A comparison of heat flow interpolations near  
subduction zones**

Buchanan C. Kerswell <sup>1</sup>Matthew J. Kohn <sup>1</sup>

<sup>1</sup>Department of Geosciences, Boise State University, Boise, ID 83725

**Key Points:**

- Inconsistent spatial patterns and variance characterize heat flow near subduction zones
- Sampling interpolations is favoured over single transects for hypothesis testing
- Future data acquisition should focus on improving interpolation quality

**Abstract**

Surface heat flow near subduction zones provides indirect observations of geodynamic processes at depth. Global heat flow databases, therefore, may test and generate hypotheses about subduction zone thermal structure and geodynamics. Here we argue that sampling from heat flow interpolations, rather than projecting discrete observations onto single trench-perpendicular transects, is a better framework for hypothesis testing. We make a direct comparison between Kriging and similarity interpolations, based on the First and Third Laws of Geography, of the most current global heat flow database and consider the implications for current geodynamic models and future subduction zone research. Inconsistent spatial patterns and variance characterize heat flow near subduction zones, regardless of interpolation method, countering hypotheses of common thermal structure (e.g. thin backarc lithospheres) and geodynamics (e.g. coupling) among subduction zones. Improving interpolations will further test current geodynamic models and should guide future data acquisitions.

**1 Introduction**

Heat escaping the solid Earth's surface indicates a dynamically cooling planet. Surface heat flow databases (Hasterok & Chapman, 2008; F. Luazeau, 2019; Pollack et al., 1993) provide a way to investigate and quantify geodynamics by relating the amount of heat escaping Earth's surface to heat-transferring and heat-generating subsurface processes such as diffusion, hydrothermal circulation, radioactive decay, fault motion, subduction dynamics, and mantle convection (Currie et al., 2004; Currie & Hyndman, 2006; Fourier, 1827; Furlong & Chapman, 2013; Yoshitsugu Furukawa, 1993; Gao & Wang, 2014; Hasterok, 2013; Kerswell et al., 2020; Parsons & Sclater, 1977; Pollack & Chapman, 1977; Rudnick et al., 1998; Carol A. Stein & Stein, 1992, 1994; Wada & Wang, 2009). Surface heat flow observations continue to motivate research, evident by more than 1,393 publications compiled in the most recent heat flow database, although the rate of publications using surface heat flow has declined since the mid 1980's (Jennings & Hasterok, 2021).

Questions such as calculating the global surface heat flux from continents and oceans require interpolating discrete heat flow observations onto a continuous approximation of Earth's surface. Interpolation attempts commonly use one or more geographic, geologic, geochronologic, or geophysical proxies to predict heat flow at unknown locations

42 by association with similar observation sites (e.g., bathymetry or elevation, proximity  
43 to active or ancient orogens, seafloor age, upper mantle shear wave velocities, David S.  
44 Chapman & Pollack, 1975; Davies, 2013; B. Goutorbe et al., 2011; W. H. Lee & Uyeda,  
45 1965; F. Lucaleau, 2019; John G. Sclater & Francheteau, 1970; Shapiro & Ritzwoller,  
46 2004). These methods are called *similarity methods* (Figure 1) and follow the assump-  
47 tions embedded in the Third Law of Geography (hereafter referred to as the Third Law):  
48 *the more similar the geographic configuration of two points, the more similar their val-*  
49 *ues* (Zhu et al., 2018).

50 Using prior information in estimation is an advantage of the Third Law and is ar-  
51 guably the most reasonable approach for interpolating surface heat flow. Our understand-  
52 ing of geodynamics and near-surface heat flow perturbations implies a strong relation-  
53 ship between surface heat flow and the set of local physical conditions (e.g., B. Goutorbe  
54 et al., 2011), irrespective of the location. For example, younger oceanic plates should have  
55 higher surface heat flow than older plates (Carol A. Stein & Stein, 1992), subducting oceanic  
56 plates will lower surface heat flow near trenches (Yoshitsugu Furukawa, 1993), and hy-  
57 drothermal circulation of seawater can modify heat escaping from oceanic crust (Has-  
58 terok et al., 2011). Interpolation by the Third Law makes reasoned predictions of heat  
59 flow with priors from many independently-tested geodynamic models. Disadvantages of  
60 the Third Law include strong bias towards geodynamic models, making determinations  
61 where, in fact, deviations from such models occur, and multiple interacting sources of  
62 uncertainty from many proxy datasets.

63 In contrast to the Third Law, there exists some degree of spatial dependence, or  
64 continuity, in the distribution of surface heat flow. A pair of surface heat flow observa-  
65 tions taken one meter apart will be strongly correlated. The correlation between pairs  
66 of observations will likely decrease with increasing distance between the pairs (Goovaerts,  
67 1997). This is encapsulated in the First Law of Geography (hereafter referred to as the  
68 First Law): *everything is related, but nearer things are more related* (Krige, 1951; Math-  
69 eron, 1963). The spatial (dis)continuity of surface heat flow represents the areal extent  
70 of geodynamic processes and their interactions. For example, patterns of consistently low  
71 surface heat flow outline the areal extent of cratons (Figure 1) and consistent patterns  
72 of heat flow near volcanic arcs are interpreted to reflect common backarc lithospheric ther-  
73 mal structures (Currie et al., 2004; Currie & Hyndman, 2006; Roy D. Hyndman et al.,

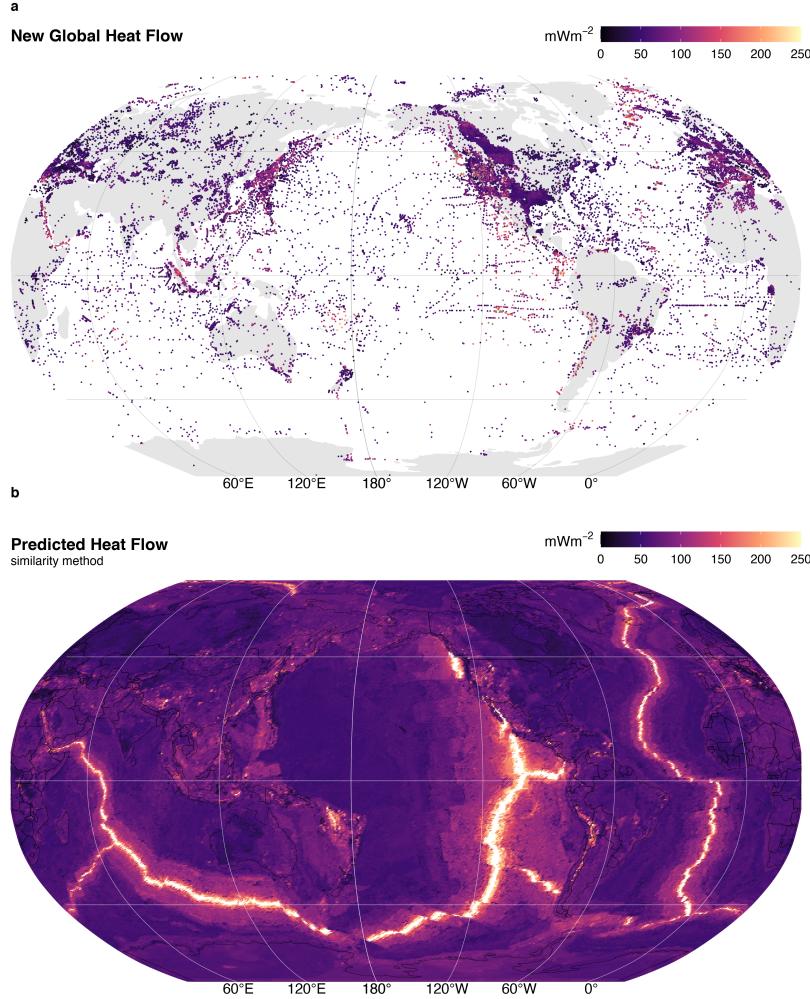


Figure 1: Global heat flow. (a) The NGHF database ( $n = 69729$ ) and (b) interpolation by similarity method. Data from Luazeau (2019).

74 2005) and slab-mantle mechanical coupling depths in subduction zones (Yoshitsugu Fu-  
75 rukawa, 1993; Kerswell et al., 2020; Wada & Wang, 2009).

76 Predicting surface heat flow by considering many nearby observations (i.e. Krig-  
77 ing, Krige, 1951) is advantageous because spatial dependence is conserved and uncer-  
78 tainty is only dependent on the distance between pairs of observations (Chiles & Delfiner,  
79 2009). However, Kriging is disadvantageous because it assumes that the underlying dis-  
80 tribution of heat flow is *stationary* (constant in space and time), which likely fails in geo-  
81 dynamically complex regions. This problem is overcome by relaxing assumptions of sta-  
82 tionarity and applying techniques that respect the Second Law of Geography: *spatial phe-*

83 *nomena are inherently heterogenous* (Goodchild, 2004), such as directional Kriging or  
84 Markov-Bayes techniques that include proxies as priors (Bárdossy, 1997).

85 In this study we attempt to answer the following questions: 1) Are global heat flow  
86 interpolations predicted by Kriging and similarity methods comparable? 2) What are  
87 the implications of the differences according to the implicit assumptions embodied in the  
88 First and Third Laws of Geography? 3) Which method is better suited for hypothesis  
89 testing? 4) How can the interpolations presented here guide future data collection ef-  
90 forts?

91 We first use ordinary Kriging to interpolate the New Global Heat Flow (NGHF)  
92 database of F. Lucaleau (2019). We then compare our interpolation results to those of  
93 F. Lucaleau (2019) and consider the implications of Kriging (First Law) vs. similarity  
94 (Third Law) methods of interpolation. We restrict our comparison to areas near sub-  
95 duction zone segments defined by Syracuse & Abers (2006) for two reasons: 1) to pro-  
96 vide heat flow interpolations and statistics useful to subduction zone research, and 2)  
97 to emphasize differences and idiosyncrasies in both interpolation approaches in a com-  
98 plex tectonic and thermal setting. We find that Kriging and similarity methods are com-  
99 parable for most subduction segments. Both interpolations show inconsistent patterns  
100 of heat flow and spatial continuity. This result implies single trench-perpendicular heat  
101 flow samples is an incomplete framework for hypothesis testing. Further, inconsistent  
102 spatial continuity and heat flow patterns counter hypotheses of common thermal struc-  
103 ture and geodynamics among subduction zones. We suggest future research focus on gen-  
104 erating high-quality interpolations and discuss considerations for data acquisition pri-  
105 orities.

## 106 2 Methods

### 107 2.1 The NGHF Database

108 The NGHF database was downloaded from the supplementary material of F. Lu-  
109 cazeau (2019). It contains 69729 data points, their locations in latitude/longitude, and  
110 metadata—including a data quality rank (Code 6) from A to D (with Code 6 = Z = un-  
111 determined). The reader is referred to F. Lucaleau (2019) for details on compilation, ref-  
112 erences, and historical perspective on the NGHF and previous compilations. We use NGFH

113 because it is the most recent database available, has been carefully compiled, and is open-  
 114 access.

115 Like F. Lucazeau (2019), we exclude 4790 poor quality observations (Code 6 = D)  
 116 from our analysis. We further remove 350 data points without heat flow observations and  
 117 two without geographic information. Multiple observations at the same location are parsed  
 118 to avoid singular covariance matrices during Kriging:

$$\begin{aligned} f(X_i^q, Y_i^q) = \\ X_i^q > Y_i^q \rightarrow z_i = x_i \\ X_i^q < Y_i^q \rightarrow z_i = y_i \\ X_i^q = Y_i^q \rightarrow z_i = RAND(x_i, y_i) \end{aligned} \quad (1)$$

119 where  $X_i^q$  and  $Y_i^q$  represent the quality of each duplicate observation pair at loca-  
 120 tion  $i$ ,  $RAND$  is a random function that selects either the observation  $x_i$  or  $y_i$ , and  $z_i$   
 121 stores the observation selected by  $f(X_i^q, Y_i^q)$ . The final dataset used for Kriging has  $n =$   
 122 55274 observations after parsing  $n = 32430$  duplicate observation.

## 123 2.2 Kriging

124 Kriging is a three-step process that involves first estimating an experimental var-  
 125 iogram,  $\hat{\gamma}(h)$ , fitting the experimental variogram with one of many variogram models,  
 126  $\gamma(h)$ , and finally using the modelled variogram to predict random variables at unknown  
 127 locations (Cressie, 2015; Krige, 1951). We use the general-purpose functions defined in  
 128 the “R” package **gstat** (Gräler et al., 2016; Pebesma, 2004) to perform all three steps.  
 129 We begin by estimating an experimental variogram as defined by Bárdossy (1997):

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{N(h)} (Z(u_i) - Z(u_j))^2 \quad (2)$$

130 where  $N(h)$  is the number of pairs of points,  $Z(u_i)$  and  $Z(u_j)$ , separated by a lag  
 131 distance,  $h = |u_i - u_j|$ . We evaluate  $\hat{\gamma}(h)$  at fifteen lag distances by binning the irreg-  
 132 ular spaced data with a bin width,  $\delta$ , equal to a proportion of the maximum lag distance,  
 133  $c$ , divided by the number of lags used to evaluate the variogram. The lag cutoff param-  
 134 eter,  $c$ , is optimized by genetic algorithm (discussed below). The binwidth is then  $\delta =$

135 max( $N(h)$ )/(15c), and  $N(h) \leftarrow N(h, \delta h) = \{i, j : |u_i - u_j| \in [h - \delta h, h + \delta h]\}$ . In simple  
 136 terms, Equation 2 represents the similarity, or dissimilarity, between pairs of observa-  
 137 tions in space. Equation 2 is adheres to the First Law of Geography and is derived from  
 138 the theory of *regionalized variables* (Matheron, 1963, 2019), which formally defines a prob-  
 139 abilistic framework for spatial interpolation of natural phenomena. It is important for  
 140 the reader to understand the fundamental assumptions implicit in Equation 2 in order  
 141 to understand the comparison of interpolation techniques discussed later. The basic as-  
 142 sumptions used in our Kriging method are:

- 143 •  $\hat{\gamma}(h)$  is directionally invariant (isotropic)
- 144 •  $\hat{\gamma}(h)$  is evaluated in two-dimensions and neglects elevation,  $Z(u) \in \mathbb{R}^2$
- 145 • The first and second moments of  $Z(u)$  have the following conditions over the do-  
     main  $D$ :

$$\begin{aligned} E[Z(u)] &= \text{mean} = \text{constant}, & \forall u \in D \\ E[(Z(u + h) - \text{mean})(Z(u) - \text{mean})] &= C(h), & \forall |u, u + h| \in D \end{aligned} \quad (3)$$

147 The last assumption (Equation 3) is called “second-order stationarity” and is im-  
 148 plicit in the First Law of Geography. It assumes the underlying probability distribution  
 149 of the random variable,  $Z(u)$ , does not change in space and the covariance,  $C(h)$ , only  
 150 depends on the distance,  $h$ , between two random variables. These assumptions are ex-  
 151 pected to be valid in cases where the underlying natural process is stochastic, spatially  
 152 continuous, and has the property of additivity such that  $\frac{1}{n} \sum_{i=1}^n Z(u_i)$  has the same mean-  
 153 ing as  $Z(u)$  (Bárdossy, 1997).

154 The following are two illustrative cases where Equation 3 is likely valid:

- 155 1. The thickness of a sedimentary unit with a homogeneous concentration of radioac-  
 156 tive elements can be approximated by  $q_s = q_b + \int A dz$ , where  $q_b$  is a constant  
 157 heat flux entering the bottom of the layer and  $A$  is the heat production within the  
 158 layer with thickness  $z$  (Furlong & Chapman, 2013). If we have two samples,  $Z(u_1) =$   
 159  $31 \text{ mW/m}^2$  and  $Z(u_2) = 30.5 \text{ mW/m}^2$ , their corresponding thicknesses would  
 160 be  $Z'(u_1) = 1000 \text{ m}$  and  $Z'(u_2) = 500 \text{ m}$  for  $A = 0.001 \text{ mW/m}^3$  and  $q_b =$   
 161  $30 \text{ mW/m}^2$ . The variable,  $Z(u)$ , in this case is additive because the arithmetic mean

162 of the samples is a good approximation of the average sedimentary layer thickness,  
 163  $(Z(u_1) + Z(u_2))/2 = 750 \text{ m}$ .

164 2. The age of young oceanic lithosphere can be approximated by  $q_s(t) = kT_b(\pi\kappa t)^{-1/2}$ ,  
 165 where  $q_s(t)$  is the surface heat flow of a plate with age,  $t$ ,  $T_b$  is the temperature  
 166 at the base of the plate,  $k$  is thermal conductivity, and  $\kappa = k/\rho C_p$  is thermal dif-  
 167 fusivity (Carol A. Stein & Stein, 1992). For  $k = 3.138 \text{ W/mK}$ ,  $\rho = 3330 \text{ kg/m}^3$ ,  
 168  $C_p = 1171 \text{ J/kgK}$ ,  $T_b = 1350^\circ\text{C}$ , two samples,  $Z(u_1) = 180 \text{ mW/m}^2$  and  $Z(u_2) =$   
 169  $190 \text{ mW/m}^2$ , would correspond to plates with ages of  $Z'(u_1) = 10 \text{ Ma}$ , and  $Z'(u_2) =$   
 170  $9 \text{ Ma}$ , respectively. Since  $Z(u_1)+Z(u_2)/2 = 185 \text{ mW/m}^2$  and  $Z'(185 \text{ mW/m}^2) =$   
 171  $9.5 \text{ Ma} = Z'(u_1) + Z'(u_2)/2$ , the variable  $Z(u)$  in this case is also additive.

172 In contrast, Equation 3 is likely invalid in regions that transition among two or more  
 173 tectonic regimes. For example, the expected heat flow  $E[Z(u)] = \text{mean}$  will change when  
 174 moving from a spreading center to a subduction zone.  $E[Z(u)] = \text{mean} \neq \text{constant}$   
 175 over the region of interest. Proceeding with Equation 3 in this case has the effect of mask-  
 176 ing the geodynamic complexity. In other words, the First Law of Geography is violated  
 177 and the geodynamic complexity will be *invisible* to Kriging predictions unless heatflow  
 178 observations are sufficiently dense. We will see that this has important implications when  
 179 comparing our Kriging method to F. Lucaleau (2019)'s interpolation method, which is  
 180 exactly opposite of this formalism—it only considers the similarities among physical prox-  
 181 ies and not spatial dependence.

182 The second step is to fit the experimental variogram with a variogram model,  $\gamma(h)$ .  
 183 In this study we fit two popular variogram models to the experimental variogram. We  
 184 use models with sill, which implies the spatial dependence between pairs of points has  
 185 a finite range. The spherical and exponential variogram models used in this study are  
 186 defined as (Chiles & Delfiner, 2009; Cressie, 2015):

$$sph \leftarrow \gamma(h) = \begin{cases} n + s \left( \frac{3h}{2a} - \frac{1}{2} \left( \frac{h}{a} \right)^3 \right), & \text{if } 0 \leq h \leq a \\ n + s, & \text{if } h > a \end{cases} \quad (4)$$

$$exp \leftarrow \gamma(h) = n + s \left( 1 - \exp \left( \frac{-h}{a} \right) \right), \quad \text{if } h \geq 0$$

187 where  $n$  is the nugget,  $s$  is the sill, and  $a$  is the effective range. The effective range,  
 188  $a$ , is related to the range,  $r$ , by  $a = r$  and  $a = r/3$  for spherical and exponential mod-

189 els, respectively (Gräler et al., 2016; Pebesma, 2004). We use the function `fit.variogram`  
 190 in `gstat` to try both variogram models. The best model is selected by the minimum mis-  
 191 fit by weighted least square (WLS, Pebesma, 2004).

192 We use ordinary Kriging for our interpolation step, which predicts the value of a  
 193 random function,  $\hat{Z}(u)$ , at unknown locations as a linear combination of all known lo-  
 194 cations in the domain,  $D$  (Bárdossy, 1997):

$$\hat{Z}(u) = \sum_{i=1}^n \lambda_i Z(u_i), \quad \forall u \in D \quad (5)$$

195 The conditions in Equation 3 set up a constrained minimization problem since one  
 196 has:

$$E[Z(u)] = \text{mean}, \quad \forall u \in D \quad (6)$$

197 The linear estimator must obey

$$E[\hat{Z}(u)] = \sum_{i=1}^n \lambda_i E[Z(u_i)] = \text{mean} \quad (7)$$

198 so the weights must be

$$\sum_{i=1}^n \lambda_i = 1 \quad (8)$$

199 This is the first constraint, also known as the unbiased condition, which states that  
 200 the sum of the weights must equal one. However, there is an infinite set of real numbers  
 201 one could use for the weights,  $\lambda_i$ . Our goal is to find the set of weights in Equation 5 that  
 202 minimizes the estimation variance. This can be solved by minimizing the covariance func-  
 203 tion,  $C(h)$  from Equation 3:

$$\begin{aligned}
\sigma^2(u) &= \text{Var}[Z(u) - \hat{Z}(u)] = E \left[ (Z(u) - \sum_{i=1}^n \lambda_i Z(u_i))^2 \right] = \\
E \left[ Z(u)^2 + \sum_{j=1}^n \sum_{i=1}^n \lambda_j \lambda_i Z(u_j) Z(u_i) - 2 \sum_{i=1}^n \lambda_i Z(u_i) Z(u) \right] &= \\
C(0) + \sum_{j=1}^n \sum_{i=1}^n \lambda_j \lambda_i C(u_i - u_j) - 2 \sum_{i=1}^n \lambda_i C(u_i - u) &
\end{aligned} \tag{9}$$

Minimizing Equation 9 with respect to the unbiased condition (Equation 8), yields the best linear unbiased estimator (BLUE, Bárdossy, 1997) for Equation 5 and together are considered the Kriging system. In our case, this is done by the function `krige` in `gstat`. We use the function `krige.cv` in `gstat` to estimate the misfit between observations and Kriging interpolations by ten-fold cross validation (Pebesma, 2004).

Further, we use a general purpose genetic algorithm, `ga`, from the R package, `GA` (Scrucca, 2013, 2017), to optimize Kriging parameters after Z. Li et al. (2018). The results from the genetic algorithm are comparable to the non-genetic-algorithm results. However, some inconsistent variogram fitting by the algorithm is suspect. We present these results and discuss their implications in sec. 8.2.

### 2.3 Map Projection and Interpolation Grid

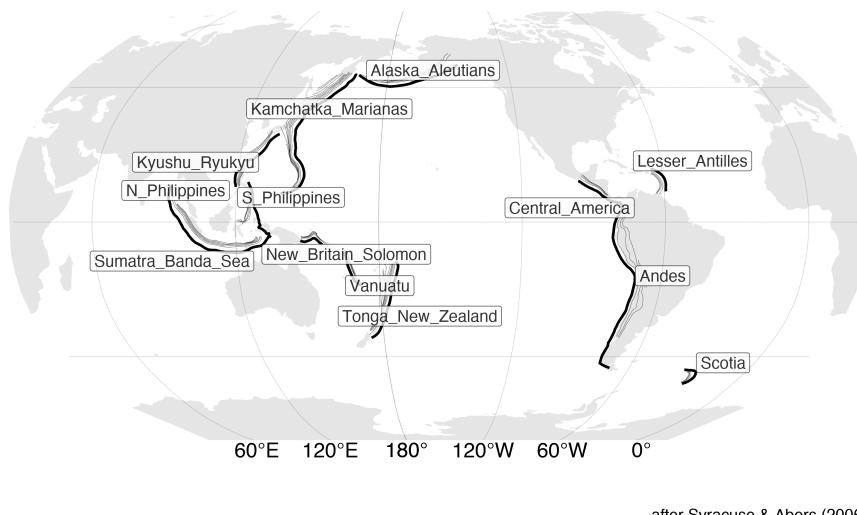
We interpolate onto the same  $0.5^\circ\text{C} \times 0.5^\circ\text{C}$  grid as F. Lucaleau (2019) so a direct difference could be calculated between our interpolation methods and F. Lucaleau (2019)'s. The NGHF and grid with predicted heat flow from F. Lucaleau (2019) were transformed into a Pacific-centered Robinson coordinate reference system (CRS) defined using the `proj` string (PROJ contributors, 2021):

```
+proj=robin +lon_0=-155 +lon_wrap=-155 +x_0=0 +y_0=0
+ellps=WGS84 +datum=WGS84 +units=m +no_defs
```

All geographic operations, including Kriging and taking the difference with F. Lucaleau (2019)'s heat flow predictions, are performed in the above CRS using the general-purpose functions in the “R” package `sf` (Pebesma, 2018). We define the Kriging domain near individual arc segments in two steps: 1) 1000 km buffers are drawn around the arc segments as defined by Syracuse & Abers (2006). 2) The bounding box of the 1000 km buffer is expanded by 10% on all sides (Figure 2). We use F. Lucaleau (2019)'s

228 grid for Kriging predictions so differences can be taken point-by-point at the exact same  
229 locations.

230 We provide the complete NGHF database (F. Lucaleau, 2019), filtered and parsed  
231 NGHF database, heat flow interpolations (from F. Lucaleau, 2019, and this study), and  
232 our code as supplementary information to support FAIR data policy (Wilkinson et al.,  
233 2016). These materials can also be retrieved from the official repository at [https://doi](https://doi.org/10.17605/OSF.IO/CA6ZU)  
234 .org/10.17605/OSF.IO/CA6ZU.

**a Subduction Zone Segments**

after Syracuse &amp; Abers (2006)

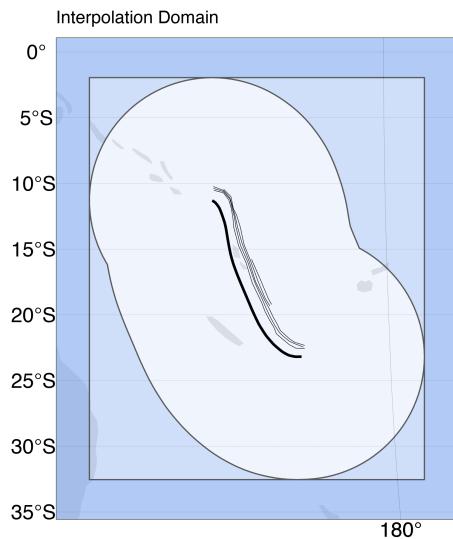
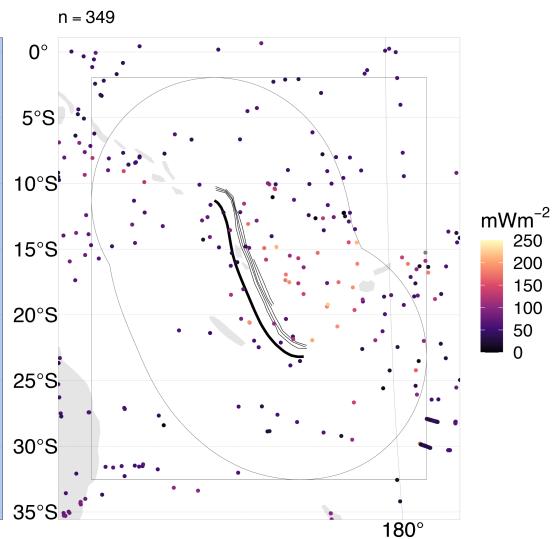
**b Vanuatu****c Vanuatu**

Figure 2: Subduction zone segments and interpolation domain. (a) Heat flow is interpolated around thirteen subduction zone segments by (b) drawing a 1000km buffer (lightest blue) around each segment and expanding the buffer's bounding box (medium blue) by 10% on all sides (darkest blue). (c) The NGHF database is cropped within the largest rectangle. Data from Syracuse & Abers (2006) and Lucaleau (2019).

235 **3 Results**236 **3.1 Heat Flow Near Subduction Zone Segments**

237 Summary statistics for surface heat flow observations by subduction zone segment  
 238 are given in Table 1 and Figure 3. Surface heat flow is median-centered around 45-70  
 239  $mWm^{-2}$  and narrowly distributed (excluding outliers) with inter-quartile ranges (IQR)  
 240 from 12 to 50  $mWm^{-2}$  for most subduction zone segments. Alaska Aleutians is the ex-  
 241 ception with a higher median of 184  $mWm^{-2}$  and broader range (IQR = 250  $mW^{-2}$ ).  
 242 The whole distributions (including outliers) for all segments are strongly right-skewed  
 243 with maximum heat flow values of several thousand of  $mWm^{-2}$  or more. Heat flow val-  
 244 ues above 250  $mWm^{-2}$  are considered geothermal areas by F. Lucaleau (2019), which  
 245 we adopt as a relevant empirical limit for anomalously high heat flow.

Table 1: Heat flow ( $mWm^{-2}$ ) observations

Segment	n	Min	Max	Median	IQR	Mean	Sigma
Alaska Aleutians	2793	4	7765	183	206	232	344
Andes	5227	7	911	45	50	87	88
Central America	5042	8	911	45	48	88	90
Kamchatka Marianas	3957	1	21700	71	48	118	548
Kyushu Ryukyu	3244	1	21700	72	44	127	604
Lesser Antilles	3535	13	1334	41	12	52	54
N Philippines	1002	3	21700	71	35	194	1051
New Britain Solomon	181	3	174	66	43	69	30
S Philippines	1444	1	21700	71	43	158	874
Scotia	72	13	145	76	23	74	28
Sumatra Banda Sea	3040	1	5600	65	47	77	120
Tonga New Zealand	506	2	416	54	40	64	45
Vanuatu	349	2	283	54	40	64	44

246 **3.2 Variogram Models**

247 The optimal variogram models and associated errors  $C_F(\Theta)$  and  $C_I(\Theta)$  are given  
 248 in Table 2. Almost twice as many experimental variograms are fit with spherical mod-

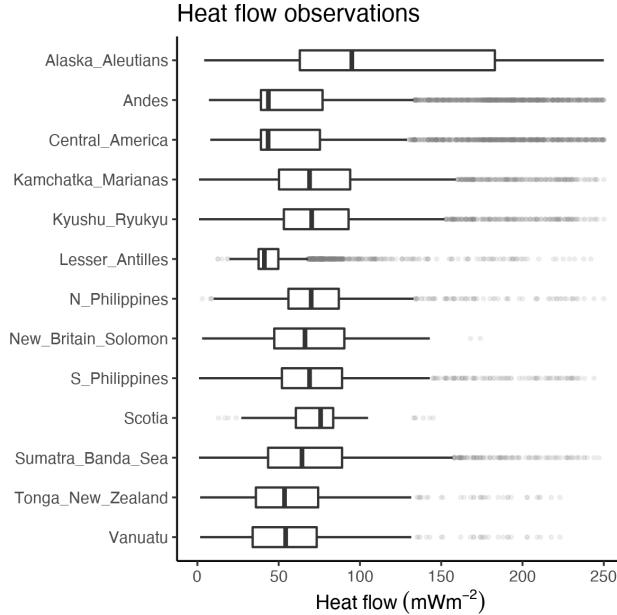


Figure 3: Distribution of heat flow observations. Heat flow near most segments is centered around  $50 \text{ mW m}^{-2}$  and highly skewed right (shadowy dot outliers). The skewness likely represents sampling near geothermal systems, volcanic arcs, or spreading centers. Data from Lucaleau (2019).

els (8) compared to exponential models (5). Variogram model sill vary substantially among the subduction zone segments between  $9$  and  $1538 \text{ mW m}^{-2}$ . Variogram model ranges also vary substantially among segments from  $4$  to  $1676 \text{ km}$ .

No apparent correlation exists between variogram model range and subduction zone segment length, number of heat flow observations, nor domain area (Figure 4). Most subduction zone segments show spatial dependence of a few hundred kilometers or less, irrespective of the number of observations or segment size. The exceptions are Kyushu Ryukyu (range =  $1774 \text{ km}$ ) and Vanuatu (range =  $573 \text{ km}$ ), whose model variogram ranges are, perhaps, anomalously high.

Table 2: Optimal varigram models

Segment	Model	Sill [ $\text{mW m}^{-2}$ ]	Range [km]
Alaska Aleutians	Sph	284	222
Andes	Sph	87	341
Central America	Sph	85	336
Kamchatka Marianas	Exp	580	277

Segment	Model	Sill [ $mWm^{-2}$ ]	Range [km]
Kyushu Ryukyu	Exp	802	864
Lesser Antilles	Exp	36	80
N Philippines	Sph	1118	240
New Britain Solomon	Exp	29	85
S Philippines	Sph	956	413
Scotia	Exp	9	4
Sumatra Banda Sea	Exp	113	32
Tonga New Zealand	Sph	47	129
Vanuatu	Sph	48	573

### 258 3.3 Interpolation Comparison

259 Summary statistics for the interpolation differences are given in Table 3 and Fig-  
 260 ure 5. Note that the difference is taken at the exact same locations for every prediction.  
 261 Differences between the similarity method and Kriging are small for most segments with  
 262 the exception of Central America, which shows a broader distribution of differences than  
 263 the other segments. The median differences range from -9 to 7  $mWm^{-2}$  with inter quar-  
 264 tile ranges from 15 to 62  $mWm^{-2}$ . Similar to the distribution of heat flow in these ar-  
 265 eas, the minimum and maximum difference in predicted heat flow are extreme and rep-  
 266 resent the failure of one method to predict extreme outliers of the other.

Table 3: Predicted heat flow ( $mWm^{-2}$ ) differences

Segment	Min	Max	Median	IQR	Mean	Sigma
Alaska Aleutians	-551	2633	-2	20	3	71
Andes	-240	2336	2	35	13	72
Central America	-241	2731	8	63	43	147
Kamchatka Marianas	-2491	297	4	15	4	39
Kyushu Ryukyu	-2492	143	6	21	2	74
Lesser Antilles	-99	589	0	16	6	32
N Philippines	-2136	284	2	24	0	65
New Britain Solomon	-80	237	1	22	5	20

Segment	Min	Max	Median	IQR	Mean	Sigma
S Philippines	-272	370	5	26	7	30
Scotia	-62	1001	-4	24	5	33
Sumatra Banda Sea	-243	385	-2	20	1	19
Tonga New Zealand	-113	1696	-9	23	-2	30
Vanuatu	-166	1657	7	27	8	40

267 Prediction differences are either approximately normally distributed, or skewed right.  
 268 Right skew and a tendency of medians to deviate positively from zero both reflect a sys-  
 269 tematic overprediction of heat flow by the similarity method compared to Kriging (Fig-  
 270 ure 5). However, Alaska Aleutians, Scotia, and Tonga New Zealand have negative me-  
 271 dian differences. While there is a tendency for the similarity method to overpredict heat  
 272 flow compared to Kriging, it is not true in every case.

273 Notable sources of prediction differences include 1) tectonic features predicted by  
 274 similarity that are absent from Kriging or 2) general discordance between the spatial con-  
 275 tinuity of heat flow observations and similarity predictions. For example, high heat flow  
 276 representing Galápagos triple junction is predicted by similarity to the SW of the Cen-  
 277 tral America segment (Figure 6 a). However, none of the triple junction arms, nor the  
 278 Galápagos hot spot, are well defined in the Kriged prediction (Figure 6 b). The inter-  
 279 polation comparison for Central America highlights two distinct regions—bright differ-  
 280 ences along the arms of the triple junction and muted agreement to the E and NE of the  
 281 Cocos Plate (Figure 6 c). Note the moderate differences within the Cocos Plate in Fig-  
 282 ure 6 a where similarity predicts high heat flow by proximity to the nearby spreading  
 283 centers, but heat flow in the region is, in fact, relatively low (compare Figure 6 a, b, c).  
 284 Similar discordance between high similarity predictions and low heat flow observations  
 285 are observed in many subduction zone segments, especially near spreading centers pre-  
 286 dicted by similarity (e.g. Figure 12; see sec. 8.1).

287 On the other side of the Caribbean Plate, near the Lesser Antilles segment, sim-  
 288 ilarity and Kriging predictions show good agreement. The Mid-Atlantic Ridge to the E  
 289 appears in both predictions (Figure 7 a, b). The spreading center is better defined with  
 290 Kriging in this case, as compared to the Galápagos triple junction, because the obser-  
 291 vational density and spatial coverage near the Lesser Antilles segment are sufficiently high

## Variogram range correlations

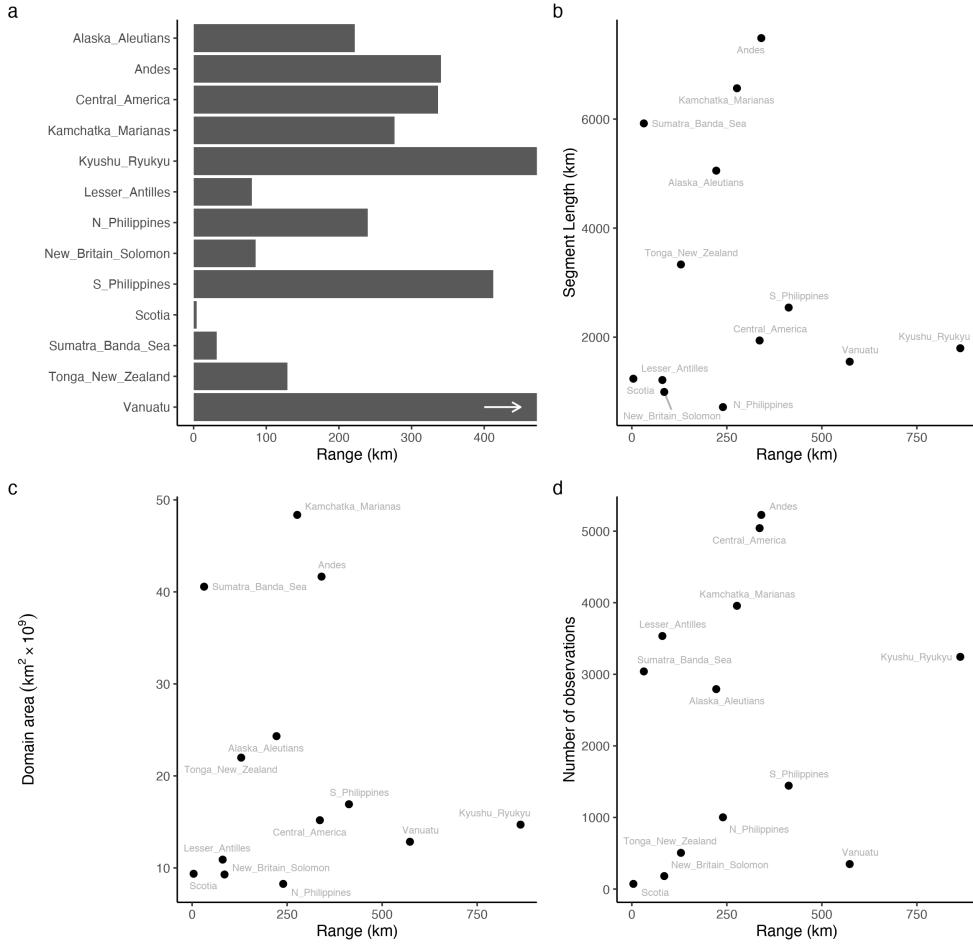


Figure 4: Summary of variogram model ranges and correlations with other features. (a) Variogram model ranges are variable, but generally below 400 km. Variogram model ranges show no correlation with segment length (b), number of heat flow observations (c), nor domain area (d). The spatial dependence of heat flow is apparently independent of these parameters.

and continuous near the Mid-Atlantic Ridge (see sec. 8.1). However, the comparison still highlight spreading centers as similarity tends to predict higher heat flow than observations.

Another example of good agreement between similarity and Kriging are interpolations near the Sumatra Banda Sea segment (Figure 8; Figure 20). Note the textural and structural complexity predicted by similarity (Figure 8 a) compared to the smooth featureless Kriging predictions (Figure 8 b). Despite the textural and structural differences, the difference between similarity and Kriging within the Sunda Plate, Australian Plate, and W Philippine Sea Plate is small (Figure 8 c).

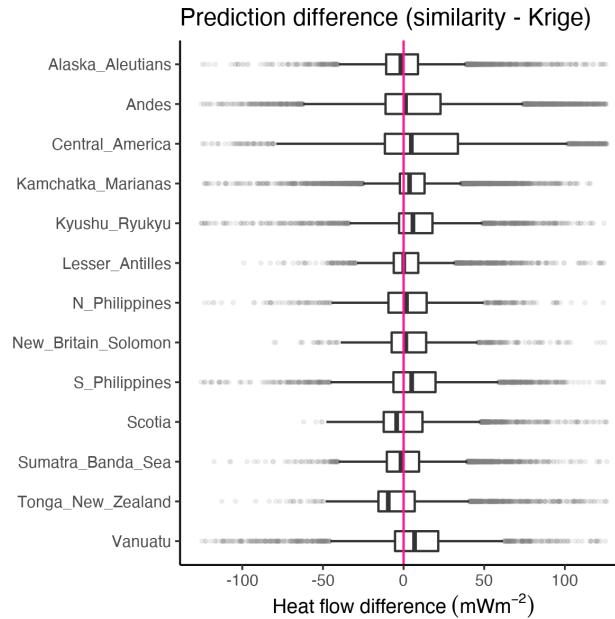


Figure 5: Point-by-point differences of predicted heat flow between similarity and Kriging interpolations. The differences for most subduction zone segments are median-centered at or near-zero with IQRs from 16 to 62. Outliers (shadowy dots) extend to extreme positive and negative differences.

Heat flow predictions near the Scotia segment illustrate a case where heat flow observations are incredibly sparse. Similarity predicts high heat flow from the East Scotia Ridge (ESR) and the WSW-ENE trending transform boundary separating the Scotia and Sandwich Plates from the Antarctic Plate (Figure 9 a). Figure 9 b appears featureless because very few heat flow observations ( $n = 72$ ) define a flat experimental variogram for all lag distances greater than four kilometers (no spatial dependence beyond 4 km, Table 2; Figure 21). Kriging predicts the expected (mean) heat flow value for the entire domain (Figure 9 b), in this case, according to Equation 5. Interestingly, the expected heat flow is a fine predictor for most of the ocean basin, except near the spreading center and transform fault (Figure 9 c). The New Britain Solomon segment shows a similar comparison (Figure 18) with good agreement between similarity and Kriging despite very few heat flow observations, little spatial dependence (small variogram range), and a featureless Kriged interpolation.

While similarity tends to define tectonic features and Kriging tends to smooth out tectonic features, we find the opposite pattern within the tectonically-complex region near Vanuatu. Similarity predicts the N-S trending spreading center separating the New Hebrides plate from the Balmoral Reef and Conway Reef microplates (Figure 10 a). How-

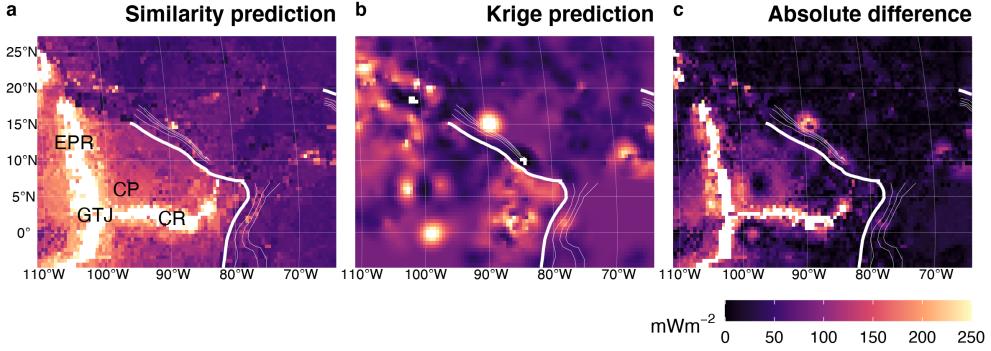


Figure 6: Similarity vs. Kriging predictions for Central America. The Galápagos triple junction (GTJ), East Pacific Rise (EPR), and Cocos Ridge (CR) are predicted by similarity (a), but not by Kriging (b). Note the moderate difference between predictions within the Cocos Plate (CP) where similarity predicts high heat flow but observations are low (c). Bold and thin white lines represent the subduction zone segment boundary and plate depth, respectively, as defined by Syracuse & Abers (2006). Heat flow data and similarity prediction from Lucaleau (2019).

318 ever, heat flow observations are sufficiently dense and continuous to partially resolve the  
 319 short ridge segments and transform faults outlining the microplates between Vanuatu  
 320 and the Tonga New Zealand segments by Kriging (Figure 10 b). The differences (Fig-  
 321 ure 10 c) are difficult to interpret because of the somewhat random discordance between  
 322 interpolation methods.

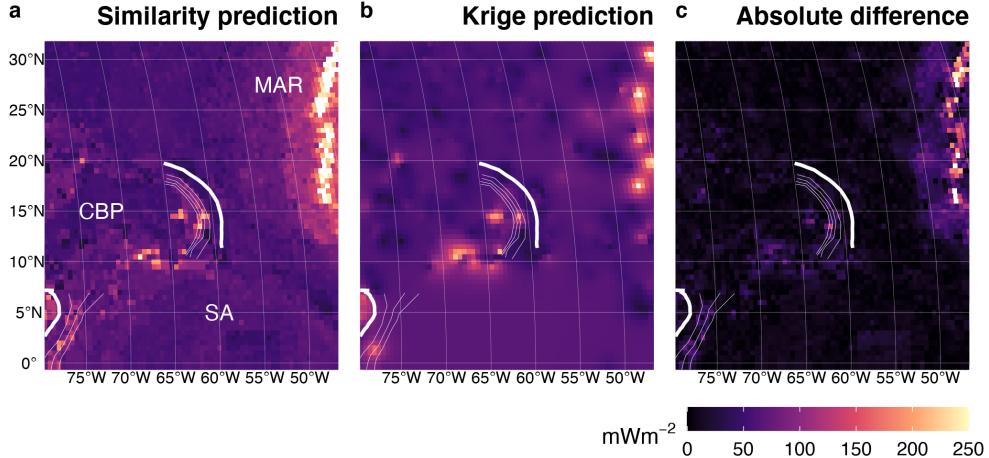


Figure 7: Similarity vs. Kriging predictions for the Lesser Antilles. The Mid-Atlantic Ridge (MAR) predicted by similarity (a) is also defined by Kriging (b) because of adequate observational density and spatial coverage near the spreading center. Good agreement between similarity and Kriging exist for the entire domain (c). CBP = Caribbean Plate, SA = South America. Bold and thin white lines represent the subduction zone segment boundary and plate depth, respectively, as defined by Syracuse & Abers (2006). Heat flow data and similarity prediction from Lucaleau (2019).

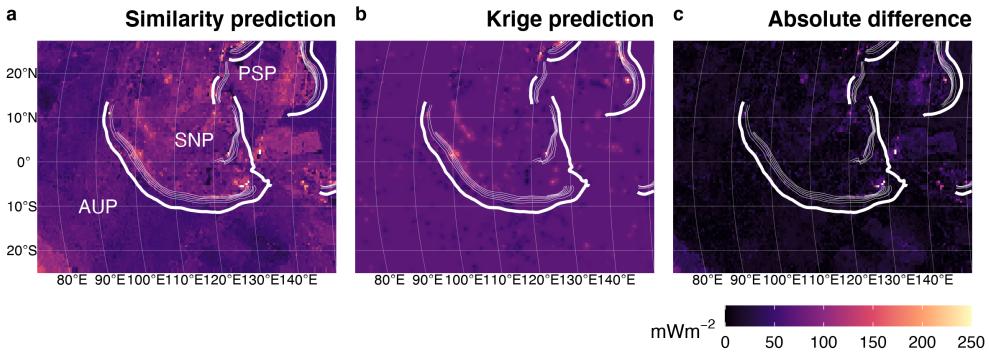


Figure 8: Similarity vs. Kriging predictions for Sumatra Banda Sea. Similarity predictions are texurally and structurally complex (a), while Kriging is smooth and featureless (b). Despite the textual and structural difference, the interpolations are similar, especially within the Sunda Plate (SNP), Australian Plate (AUP) and W Philippine Sea Plate (PSP). Bold and thin white lines represent the subduction zone segment boundary and plate depth, respectively, as defined by Syracuse & Abers (2006). Heat flow data and similarity prediction from Lucaleau (2019).

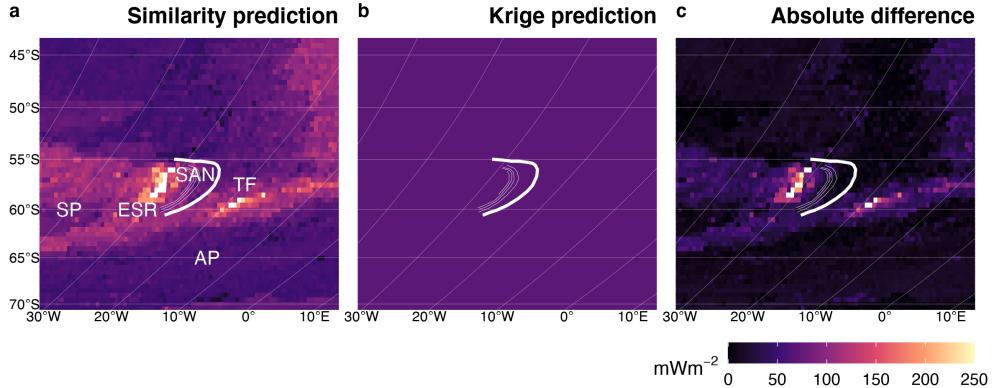


Figure 9: Similarity vs. Kriging predictions for Scotia. (a) Similarity predicts high heat flow for two tectonic features, the East Scotia Ridge (ESR) and a transform fault (TF) separating the Scotia and Sandwich Plates (SP, SAN) from the Antarctic Plate (AP). Kriging (b) is featureless because of incredibly sparse data. Despite few heat flow observations. Kriging predictions are only significantly different than similarity predictions near the ESR and transform fault (c). Bold and thin white lines represent the subduction zone segment boundary and plate depth, respectively, as defined by Syracuse & Abers (2006). Heat flow data and similarity prediction from Lucazeau (2019).

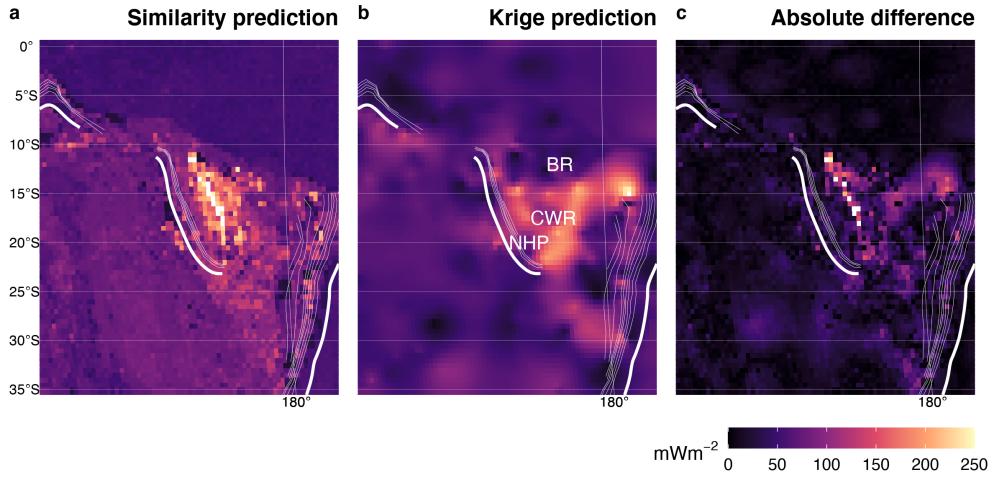


Figure 10: Similarity vs. Kriging predictions for Vanuatu. (a) Similarity resolved the spreading center separating the New Hebrides Plate (NHP) from the Balmoral Reef (BR) and Conway Reef (CR) microplates. Sufficient heat flow observations allow Kriging to resolve additional ridge segments and transform faults outlining BR and CR (b). The difference between similarity and Kriging (c) is discordant and difficult to interpret. Bold and thin white lines represent the subduction zone segment boundary and plate depth, respectively, as defined by Syracuse & Abers (2006). Heat flow data and similarity prediction from Lucazeau (2019).

323 **4 Discussion**324 **4.1 The First and Third Laws of Geography**

325 The Third Law of Geography states that *two points with similar geographic con-*  
 326 *figurations should have similar values.* In the context of heat flow near subduction sys-  
 327 *tems and associated spreading centers, the Third Law produces interpolations that high-*  
 328 *light discrete tectonic features (spreading centers and large fault systems) with complex*  
 329 *regional texture. At first glance the textural complexity may be misconstrued as real-*  
 330 *istic interpolations, but is merely an artifact of the similarity method. The texture pre-*  
 331 *dicted by similarity is artificial insofar as it does not represent spatial changes in sur-*  
 332 *face heat flow. Rather each prediction location represents an independent assignment*  
 333 *of heat flow by association to all other locations with similar geographic configurations*  
 334 *(B. Goutorbe et al., 2011; F. Lucaleau, 2019; Zhu et al., 2018).* The extent to which sim-  
 335 *ilarity predictions represent real changes of heat flow in space is entirely dependent on*  
 336 *the reliability of the Third Law, the quality of the physical proxies, and the selected com-*  
 337 *bination of proxies used for interpolation.*

338 We note a few inconsistencies with F. Lucaleau (2019)'s similarity predictions in  
 339 the domains considered in this study. First, F. Lucaleau (2019)'s predictions system-  
 340 atically overpredict heat flow near spreading centers, justifying an adjustment to their  
 341 algorithm. Second, known tectonic features within the tectonically-complex region near  
 342 Vanuatu may be better resolved by Kriging than F. Lucaleau (2019)'s predictions. It  
 343 is important to note, however, that Vanuatu is the only case where Kriging resolves tec-  
 344 tonic features that similarity does not; the trend is otherwise opposite. Moreover, the  
 345 inconsistencies near Vanuatu do not imply algorithmic issues and can likely be resolved  
 346 by similarity using a finer-scale grid.

347 The more important inconsistencies are general discordance between similarity pre-  
 348 dictions and observations. Disagreements with observations imply failures of the Third  
 349 Law, which are not easily correctable algorithmically. Cross-validation statistics given  
 350 by F. Lucaleau (2019) demonstrate good agreement with observations in general. The  
 351 cross-validation error may be sufficiently small for calculating global heat flux and prob-  
 352 ing other relevant questions on the global scale. However, testing hypotheses which re-  
 353 quire sampling heat flow on the subduction zone segment scale should carefully consider

354 where predictions and observations differ, regardless of the interpolation method (dis-  
355 cussed further below).

356 Unlike the Third Law, the First Law of Geography by definition does not allow dis-  
357 cordance between predictions and observations. This fact can be colloquially stated as  
358 *everything is related, but nearer things are more related (and points at the exact same*  
359 *location are perfectly related)*. More formally, the covariance of two points at the same  
360 location must be zero. Comparing the First and Third Laws reveals further asymmetry  
361 in the sources of errors. Sources of interpolation error include: 1) quality of heat flow  
362 observations (First & Third Law), 2) variance of predictions at unknown locations (First  
363 & Third Law), 3) residuals of predictions at known locations (Third Law), 4) Kriging  
364 weights (variogram model; First Law), 5) variances of physical proxies (Third Law), 6)  
365 combinations of physical proxies (Third Law), 7) similarity weights (similarity model;  
366 Third Law). Interpolation uncertainty is easier to conceptualize and quantify for First  
367 Law interpolations than Third Law interpolations.

368 Arguments in favour of First or Third Law interpolations, however, are not eas-  
369 ily generalized. Third Law interpolations are justified in cases with inadequate heat flow  
370 observations (e.g. Scotia and New Britain Solomon). First Law interpolations are arguably  
371 more favourable in all cases with adequate heat flow observations because 1) enough ob-  
372 servations will resolve important features, 2) spatial dependency is respected, and 3) there  
373 are fewer sources of uncertainty. However, it is difficult to know what “adequate” ob-  
374 servational density and spatial coverage are *a priori*. In any case, it may not be feasi-  
375 ble to achieve adequate observational density and spatial coverage due to time and bud-  
376 get constraints. Therefore, hypotheses and sampling strategies should be constructed with  
377 careful consideration of whether First or Third Law interpolations are more appropri-  
378 ate on a case-by-case basis.

379 Regardless of the methodology, the present interpolations show inconsistent pat-  
380 terns of heat flow and spatial variance, implying either 1) disorganized subsurface ther-  
381 mal structure, 2) spatially heterogeneous dynamics, or 3) broad obfuscation of subsur-  
382 face thermal structure and dynamics by near-surface processes. Therefore we encourage  
383 a more antireductionist view of subduction zone dynamics. We point out that while test-  
384 ing of many important subduction-related questions may not be feasible with the cur-

385 recent global database, the idea of broad dynamic commonality among subduction systems  
386 does not hold up to scrutiny from the heat flow interpolations presented here.

387 **4.2 Hypothesis Testing**

388 Testing hypotheses relating to subduction dynamics require sampling of heat flow  
389 in order to apply statistical models. Sampling in previous work commonly uses a three-  
390 part strategy: 1) draw a cross-section line perpendicular to the trench, 2) draw a rect-  
391 angle with arbitrary width bisected by the section line, 3) gather all heat flow observa-  
392 tions within the rectangle and project them onto the section line (e.g., Currie et al., 2004;  
393 Currie & Hyndman, 2006; Roy D. Hyndman et al., 2005; Wada & Wang, 2009). This sam-  
394 pling strategy is simple and most effective if measurements along section lines are equally  
395 spaced with high spatial density. Observations along straight transects perpendicular to  
396 trenches, however, are rare in the NGHF except for a few studies e.g. near the Lesser An-  
397 tilles and Sumatra Banda Sea segments, ??, (F. Lucaleau, 2019). There are additional  
398 limitations to this method, including: 1) the method increasingly violates the First Law  
399 as the size of the sampling rectangle increases—projecting more disparate points onto  
400 the section line—and 2) sampling must be repeated many times along strike to fully char-  
401 acterize the spatial distribution of heat flow near subduction zone segments. Despite these  
402 limitations, previous work use single transects to characterize whole subduction zones,  
403 which are then compared to make broad claims about global subduction dynamics (e.g.,  
404 Currie et al., 2004; Currie & Hyndman, 2006; Roy D. Hyndman et al., 2005; Kerswell  
405 et al., 2020; Wada & Wang, 2009).

406 Hypotheses such as common depths of slab-mantle mechanical coupling and com-  
407 monly thin backarc lithospheres (Currie et al., 2004; Currie & Hyndman, 2006; Yoshit-  
408 sugu Furukawa, 1993; Kerswell et al., 2020; Wada & Wang, 2009) cannot be adequately  
409 tested using the single-transect method described above. First and Third Law interpo-  
410 lations show that spatial variance in heat flow near subduction zone segments is simply  
411 too high to support any claim that subduction dynamics are operating on vastly sim-  
412 ilar spatiotemporal scales either within or among subduction zone segments. For exam-  
413 ple, sampling along section lines offset at 50 km from previously published section lines  
414 (Currie et al., 2004; Currie & Hyndman, 2006; Yoshitsugu Furukawa, 1993; Wada & Wang,  
415 2009) is unlikely to reproduce results. Insofar as heat flow can reliably answer questions  
416 about subduction zone dynamics in space and time, hypothesis must be qualified with

417 sampling techniques that consider the appropriate number of dimensions for the ques-  
 418 tion being asked. Sampling and projection onto a one-dimensional section line is insuf-  
 419 ficient for testing hypotheses about the two-dimensional distribution of dynamic processes.

420 **4.3 Heat Flow Sampling Strategies**

421 With a comparison of two approaches and interpolations, important questions may  
 422 be considered:

- 423 1. Is collecting more heat flow data necessary for future subduction zone research?  
 424 2. Where should data collection efforts be focused?  
 425 3. Should First or Third Law interpolations be favoured when prioritizing data col-  
 426 lection targets?

427 More data collection is unequivocally conducive to deeper understanding of sub-  
 428 duction zone dynamics. Assuming inexpensive and rapid raster acquisition of marine and  
 429 terrestrial heat flow is far in the future, discrete data collection from probes and bore-  
 430 holes remain the primary methods of collection. Below we discuss reasonable strategies  
 431 for data collection without making concrete recommendations. We hope the reader is  
 432 convinced by now that two-dimensional interpolations of heat flow are preferred for test-  
 433 ing hypotheses regarding geodynamics near subduction zones. Therefore, the focus of  
 434 future data collection efforts should be production of high-quality interpolations in these  
 435 regions. Strategies for producing higher-quality and higher-resolution interpolations de-  
 436 pends on the method, so a decision must first be made to use Kriging (First Law), sim-  
 437 ilarity (Third Law), or another method (e.g. Second Law).

438 Kriging interpolation quality scales with spatial density of observations. High-density,  
 439 grid-like surveys across the forearc and backarc regions are likely to yield good results.  
 440 Regularly-spaced grids are preferred over single transects because an infinite number  
 441 of transects can be sampled from a high-quality interpolation. Grid spacing should not  
 442 exceed the ranges given in Table 2. Careful avoidance of potential near-surface pertur-  
 443 bations should be prioritized over regular spacing if possible.

444 Surveying heat flow is temporally, energetically, and monetarily expensive. We sug-  
 445 gest prioritizing small segments like Scotia, the Lesser Antilles, and New Britain Solomon  
 446 as Kriging targets because they currently have few observations and their relatively lengths

allow for denser surveying. An alternative strategy is to choose a segment with existing high-density coverage and survey within observational gaps. Regular spacing is less important in the latter case.

Similarity interpolation quality depends on the combination of physical proxies and their associated heat flow distributions used in the similarity algorithm (B. Goutorbe et al., 2011; F. Lucaleau, 2019). Therefore, the quality of similarity interpolations scale with the quality of the proxy datasets. A decision must first be made on the best combination of proxy datasets, followed by careful scrutiny of the quality of the dataset. B. Goutorbe et al. (2011) provides relevant datasets with measures of each dataset's effect on a global heat flow interpolation. Datasets with the strongest degradation effects (removing them from the interpolation algorithm leads to less accurate results), such as topography, lithospheric thickness, and velocity structure (B. Goutorbe et al., 2011), should be used in future algorithms and prioritized for quality control and improvement. The cost-benefit of improving proxy datasets varies among datasets. Some datasets, like topography, are relatively easy to improve through quality control and remote acquisition, whereas improving other datasets, like lithospheric heat production or lithospheric thickness, are more involved. Contending with numerous datasets and sources of uncertainty (discussed above) make improvements to Third Law interpolations challenging.

Simple Kriging methods are comparable to similarity methods for interpolating heat flow near subduction zone systems according to Figure 5 and Table 3. Improvements to Kriging interpolations will likely outpace similarity methods with focused surveying of specific segments because high-density surveying, although costly, is more straightforward than simultaneously improving many proxy datasets. Coincidentally, high-density sampling improves similarity interpolations because any addition of high-quality measurements incrementally improves existing proxy datasets. Therefore, we suggest strategies for future heat flow acquisitions favour First Law interpolations and focus on high-density surveying of one priority segment at a time. In principle this strategy generates reliable First Law interpolations while making incremental improvements to Third Law interpolations.

**476 5 Conclusions**

477 This study uses Kriging to interpolate the New Global Heat Flow database (F. Lu-  
478 cazeau, 2019) and makes a direct comparison between Kriging and similarity (F. Lucazeau,  
479 2019) interpolations near subduction zone segments. The differences between interpo-  
480 lations highlight four important points of consideration:

- 481 1. Inconsistent patterns of heat flow and spatial variance characterize most subduc-  
482 tion zone segments, countering hypotheses of common thermal structure or geo-  
483 dynamics (e.g. coupling depths)
- 484 2. Kriging and similarity interpolation methods produce similar results near subduc-  
485 tion zone segments
- 486 3. For testing hypotheses regarding thermal structure and geodynamics, sampling  
487 from two-dimensional interpolations is favoured over gathering and projecting dis-  
488 crete observations onto single-transects
- 489 4. Focused improvements to heat flow interpolations is encouraged to test current  
490 hypotheses and advance subduction zone research
- 491 5. Improving Kriging (First Law) interpolations through focused surveys within pri-  
492 ority subduction zone segments is a favourable strategy for future data acquisi-  
493 tion

**494 6 Open Research**

495 All data, code, and heat flow interpolations can be found at <https://doi.org/10.17605/OSF.IO/CA6ZU>,  
496 the official Open Science Framework data repository. All code is MIT Licensed and free  
497 for use and distribution (see license details).

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610 **8 Appendix**611 **8.1 Heat flow observations and predictions (non-GA)**

612 The following figures are a complete set of compositions showing heat flow obser-  
 613 vations, variograms, Kriged interpolations, similarity interpolations from F. Lucaleau  
 614 (2019), and interpolation differences for each subduction zone segment. The variograms  
 615 in this section were not fit using the genetic algorithm (described in sec. 8.2) and cor-  
 616 respond to the interpolation results presented in the main text.

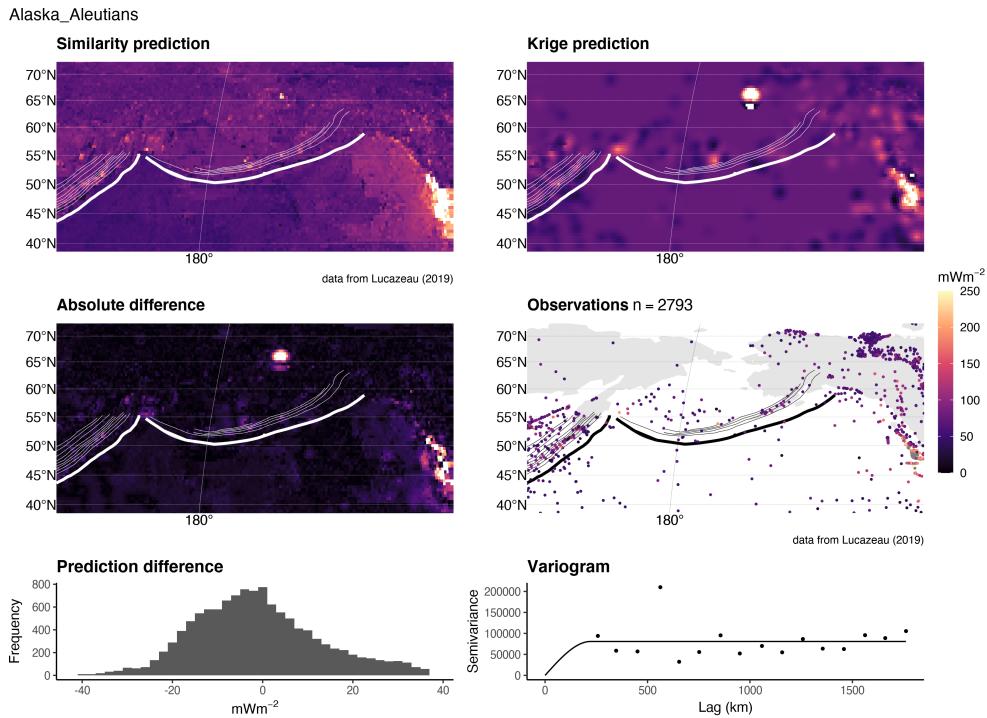


Figure 11: Similarity vs. Kriging predictions for Alaska Aleutians.

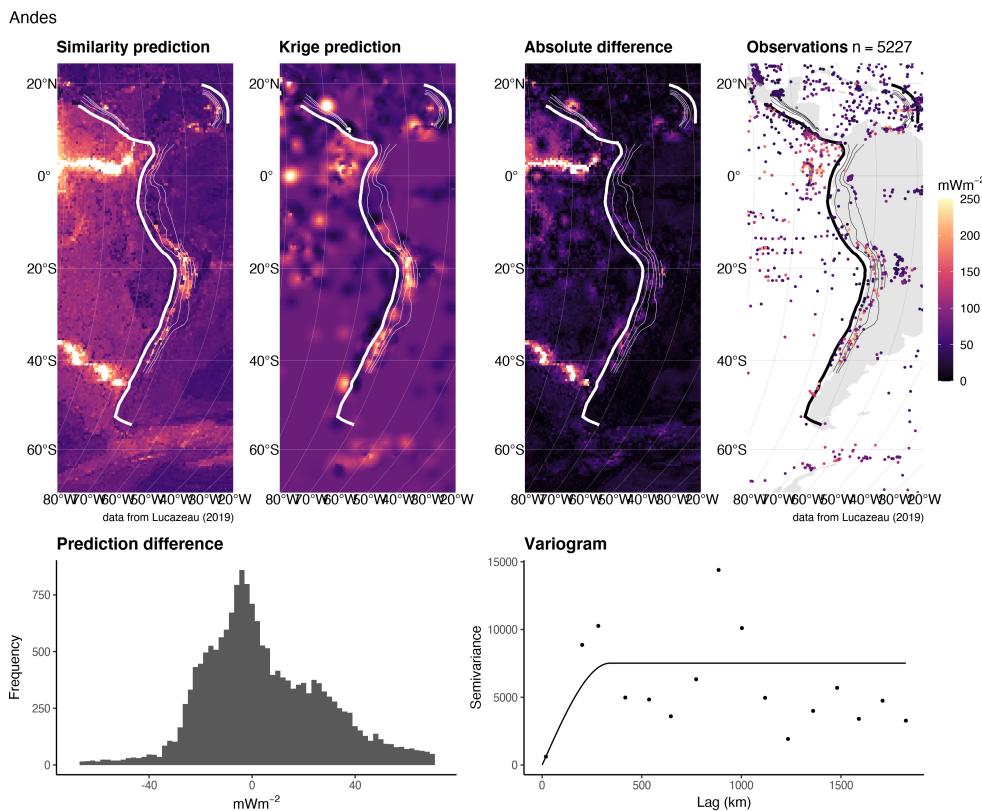


Figure 12: Similarity vs. Kriging predictions for the Andes.

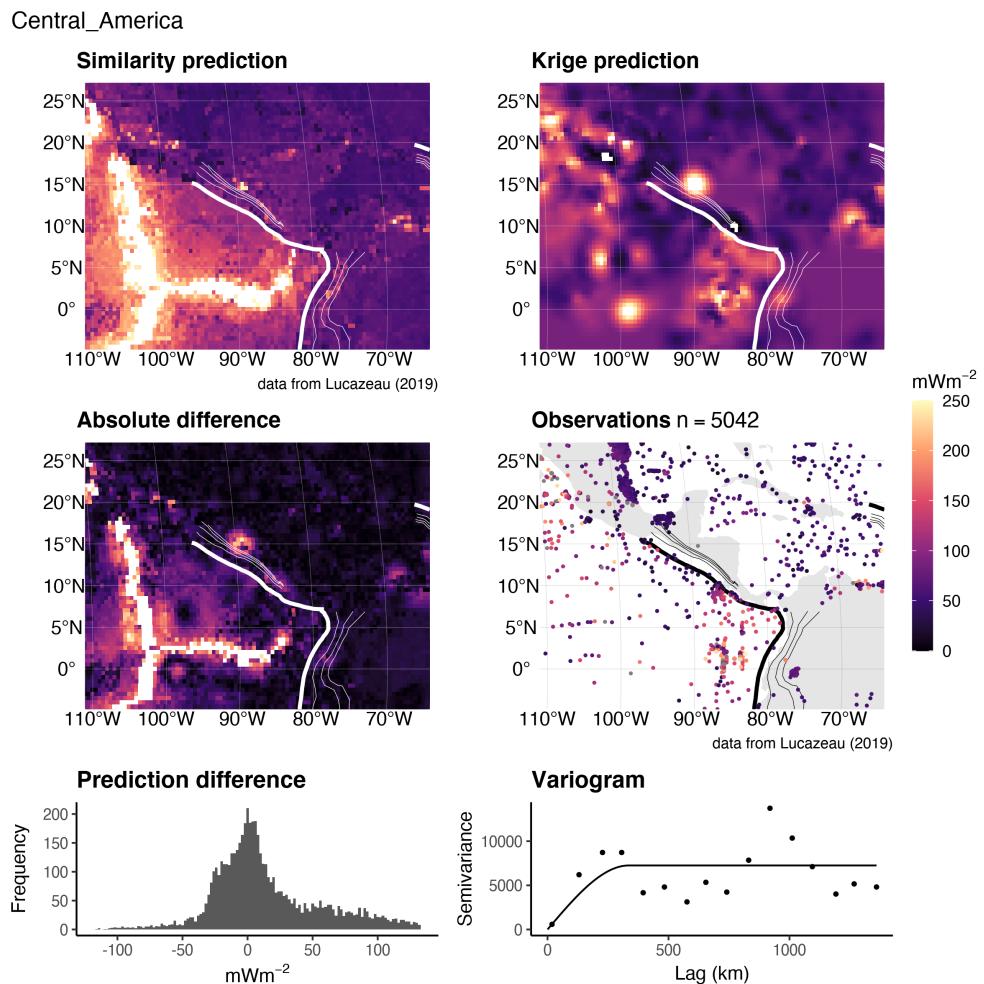


Figure 13: Similarity vs. Kriging predictions for Central America.

## Kamchatka\_Marianas

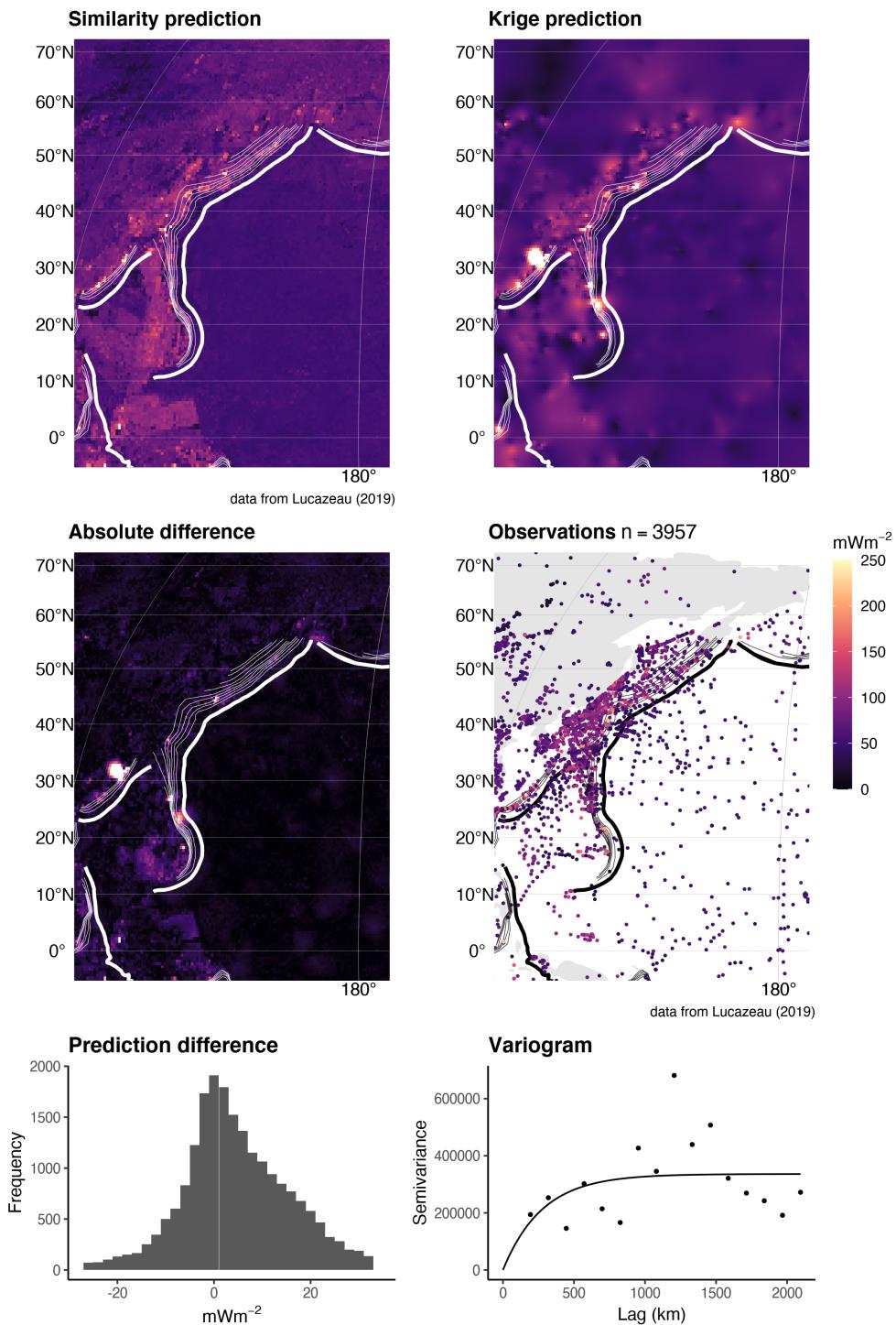


Figure 14: Similarity vs. Kriging predictions for Kamchatka Marianas.

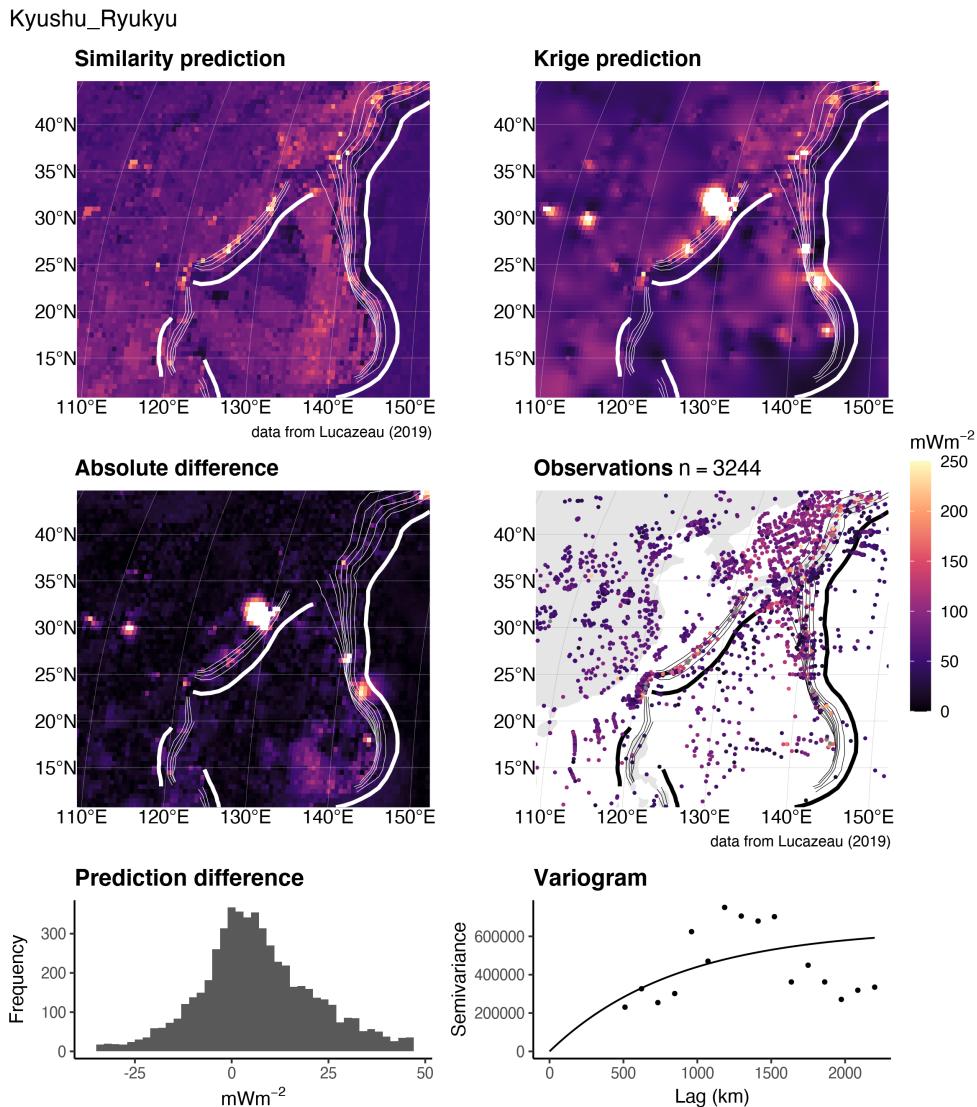


Figure 15: Similarity vs. Kriging predictions for Kyushu Ryukyu.

## Lesser\_Antilles

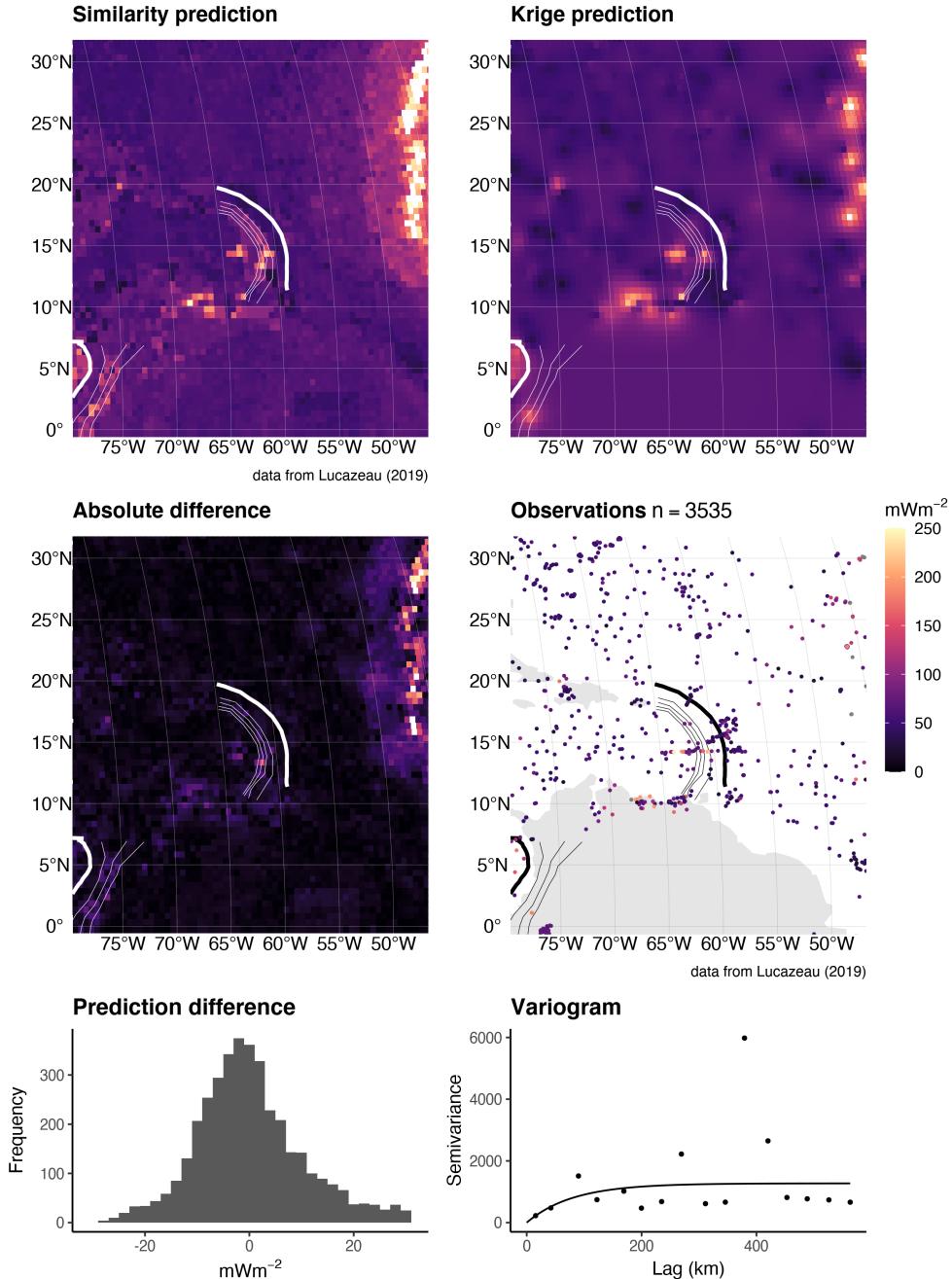


Figure 16: Similarity vs. Kriging predictions for the Lesser Antilles.

N\_Philippines

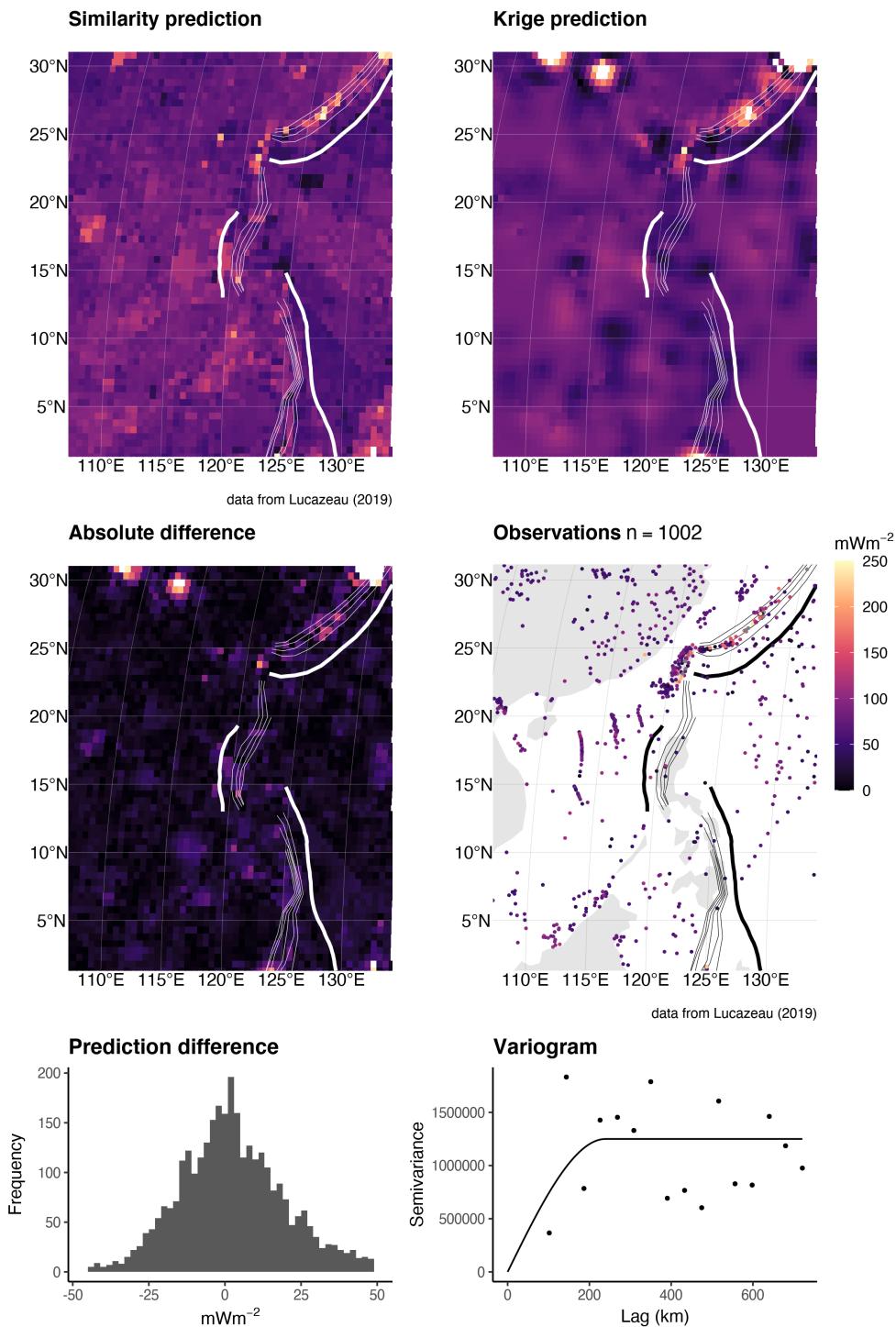


Figure 17: Similarity vs. Kriging predictions for N. Philippines.

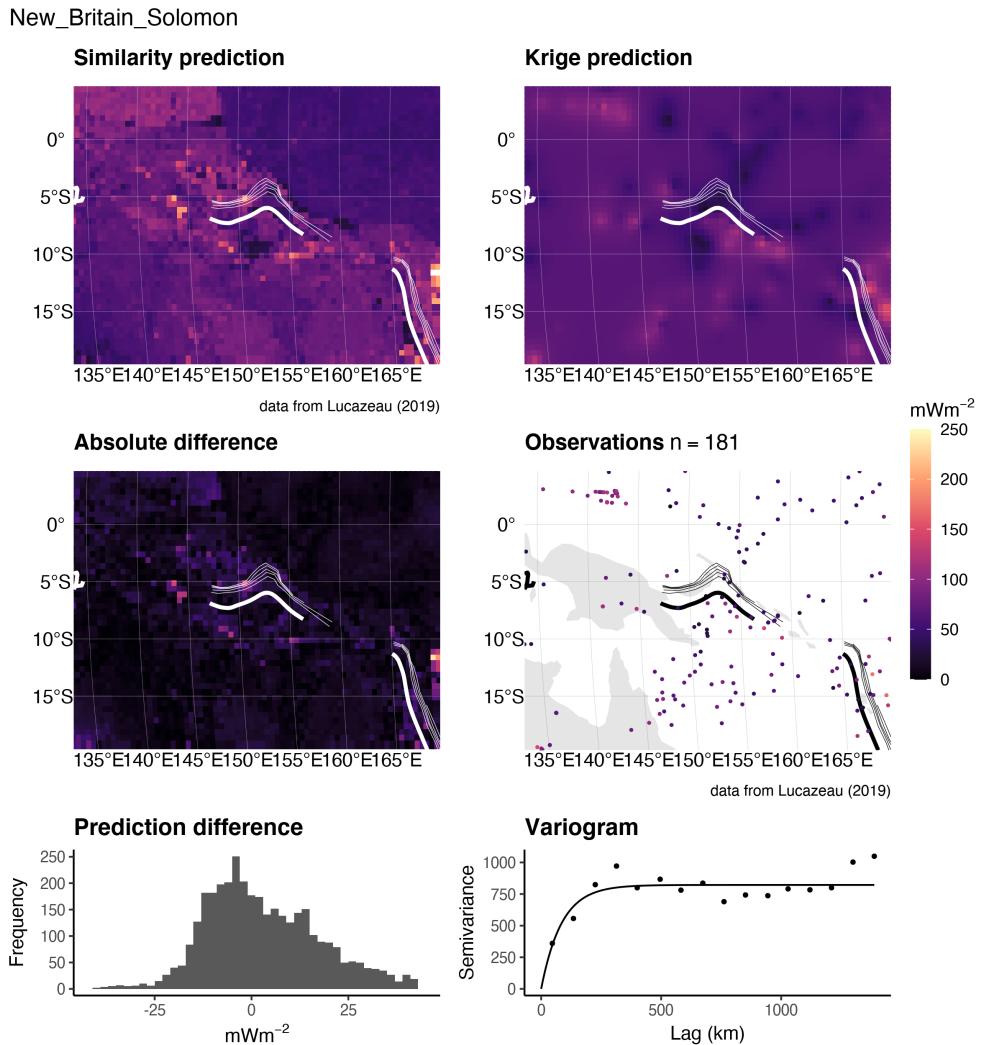


Figure 18: Similarity vs. Kriging predictions for New Britain Solomon.

S\_Philippines

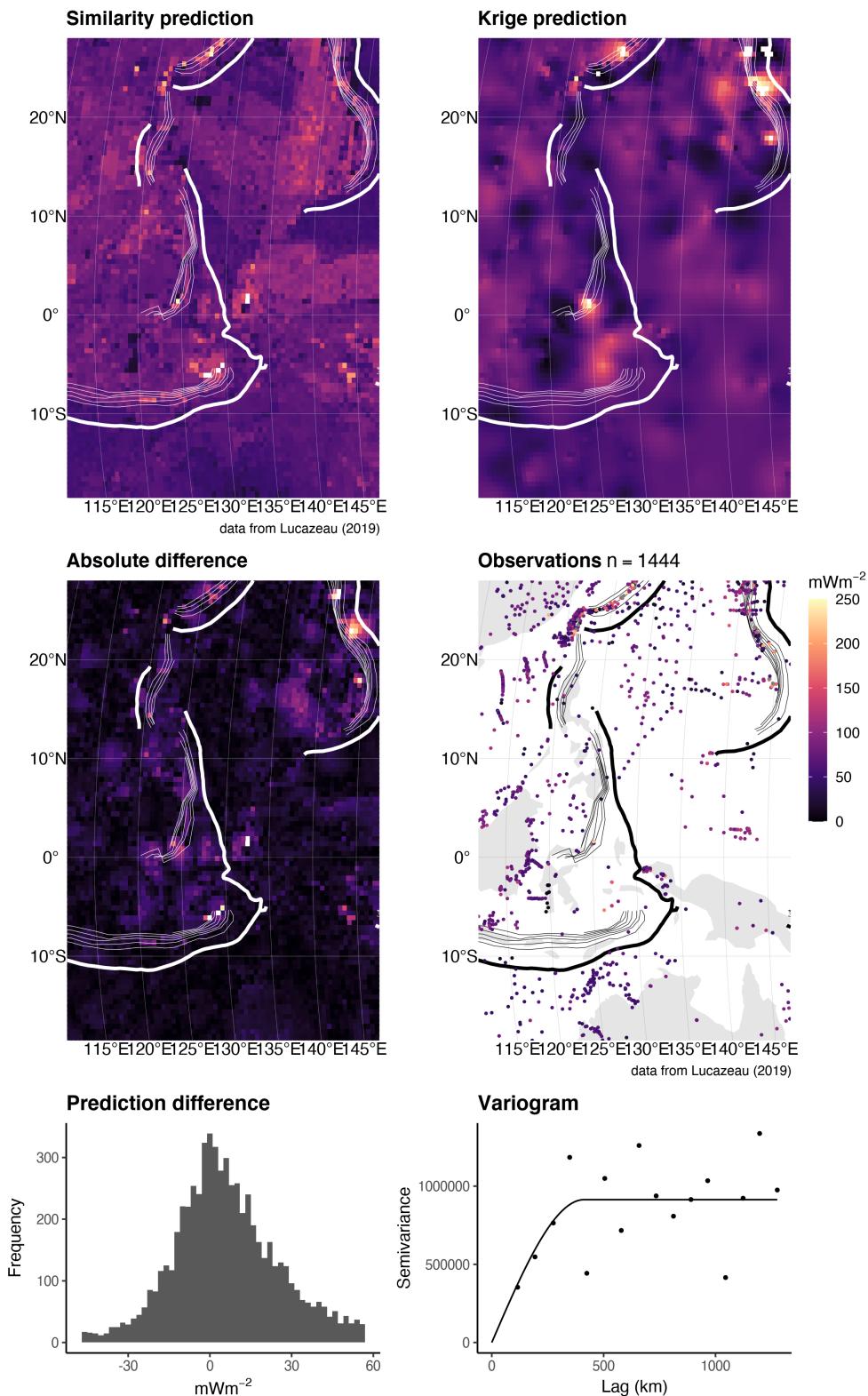


Figure 19: Similarity vs. Kriging predictions for S. Philippines.

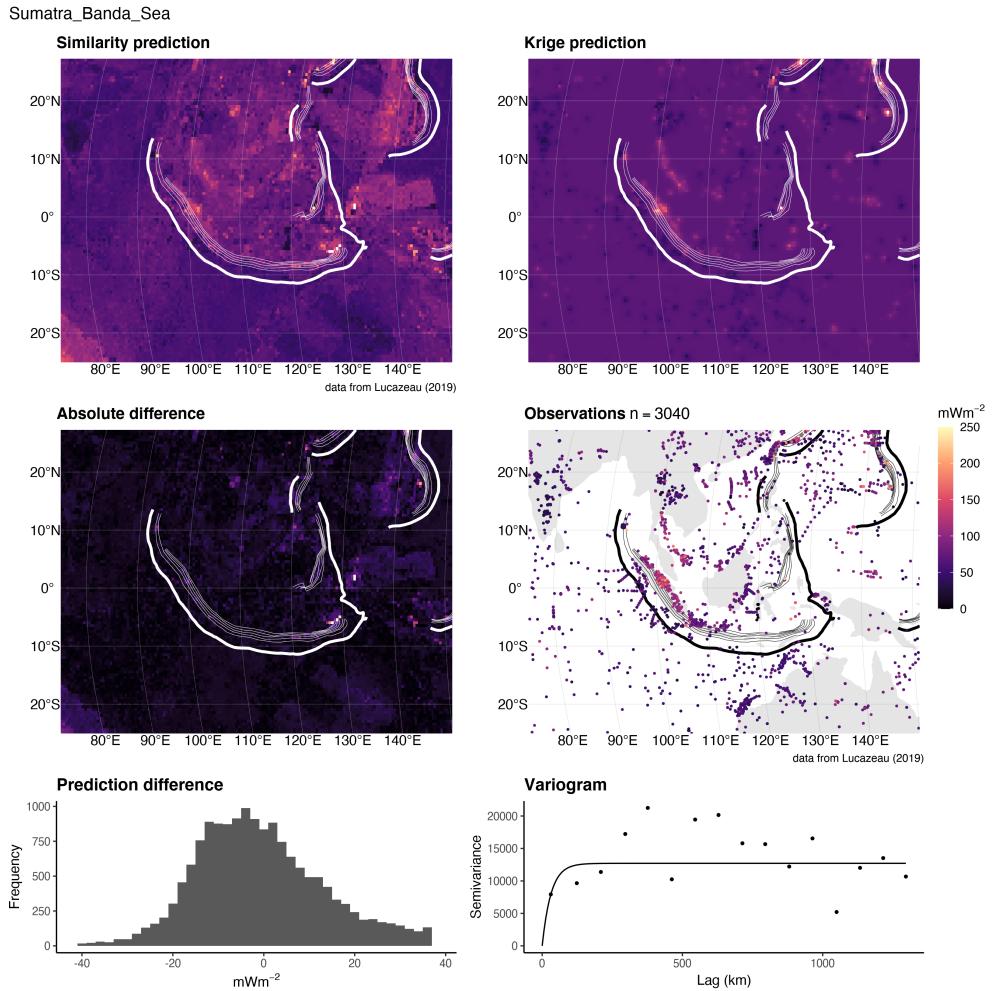


Figure 20: Similarity vs. Kriging predictions for Sumatra Banda Sea.

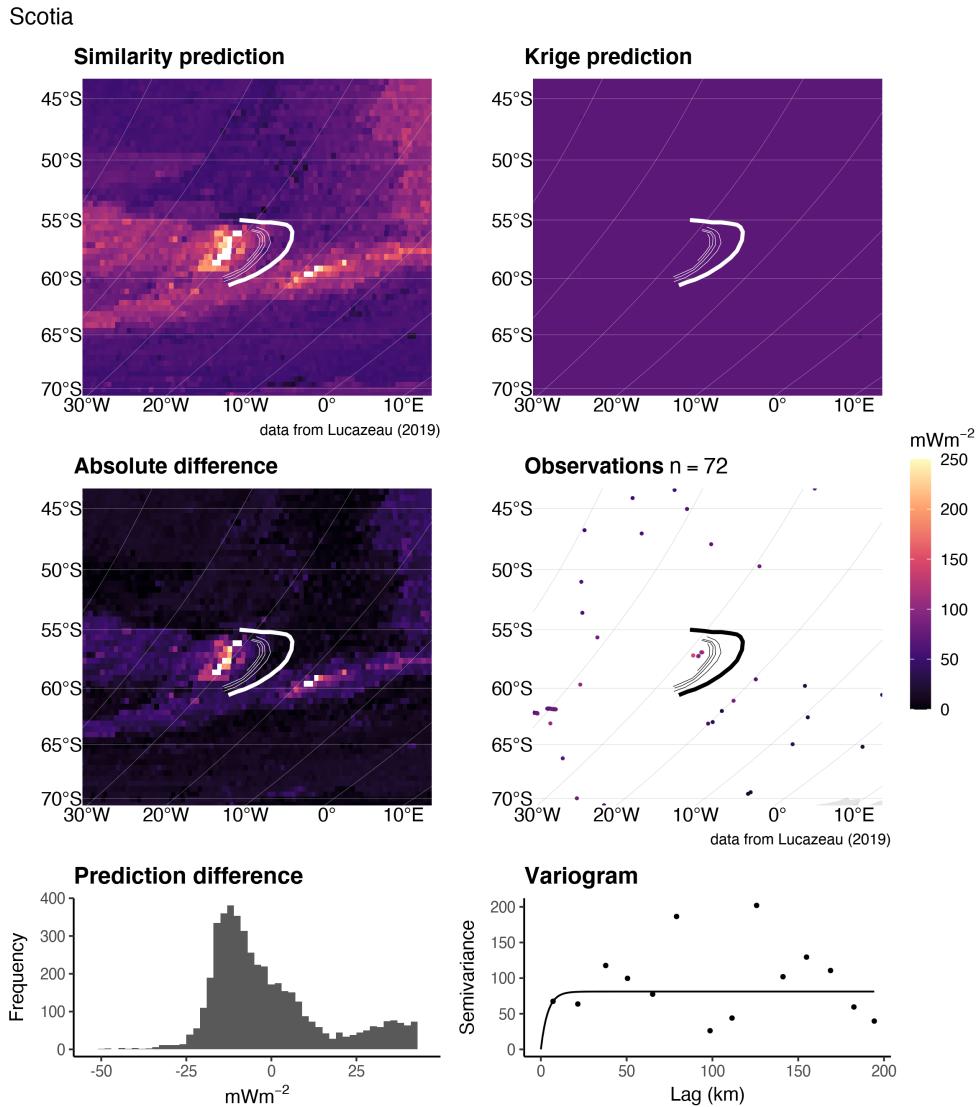


Figure 21: Similarity vs. Kriging predictions for Scotia.

Tonga\_New\_Zealand

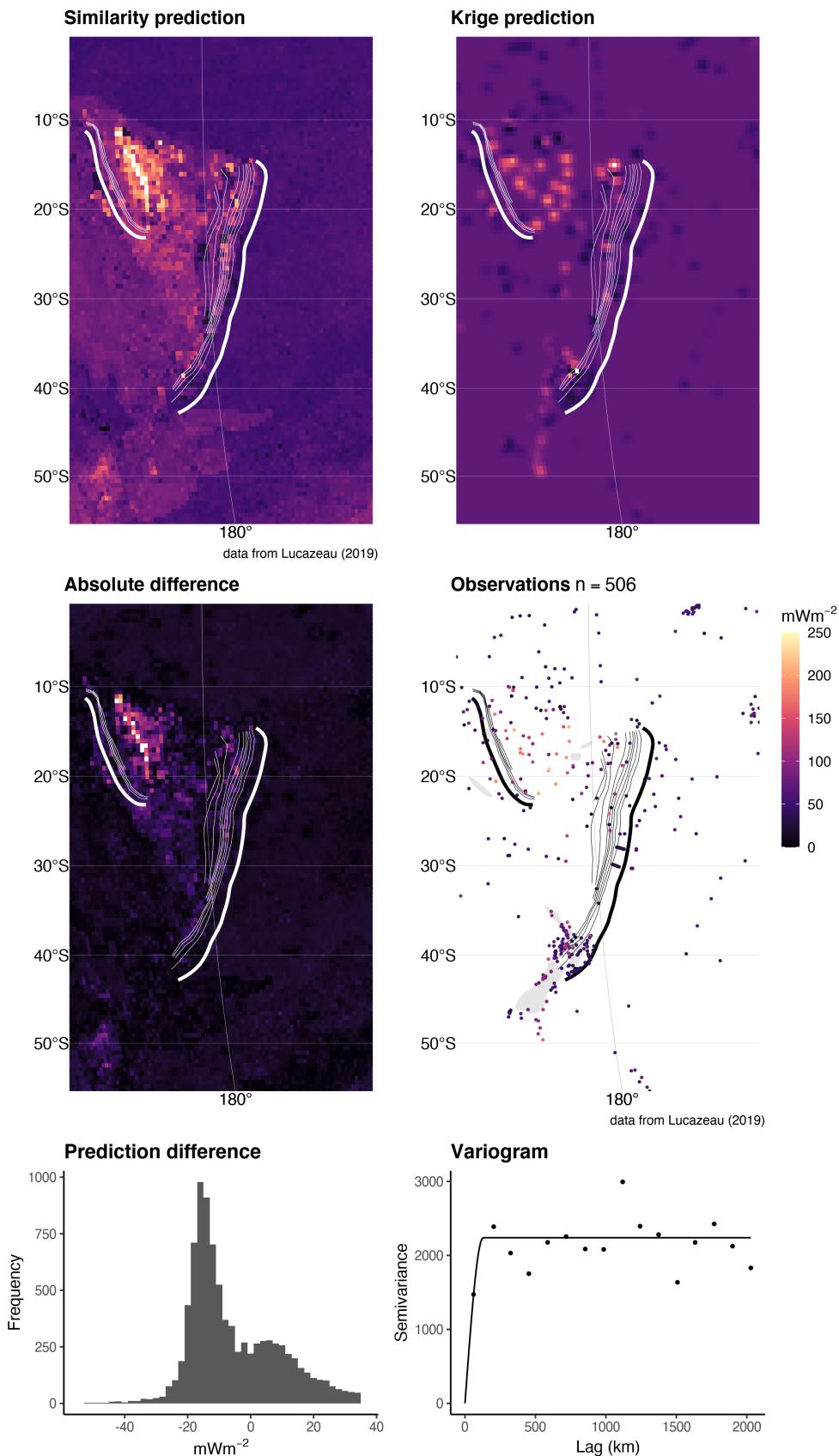


Figure 22: Similarity vs. Kriging predictions for Tonga New Zealand.

Vanuatu

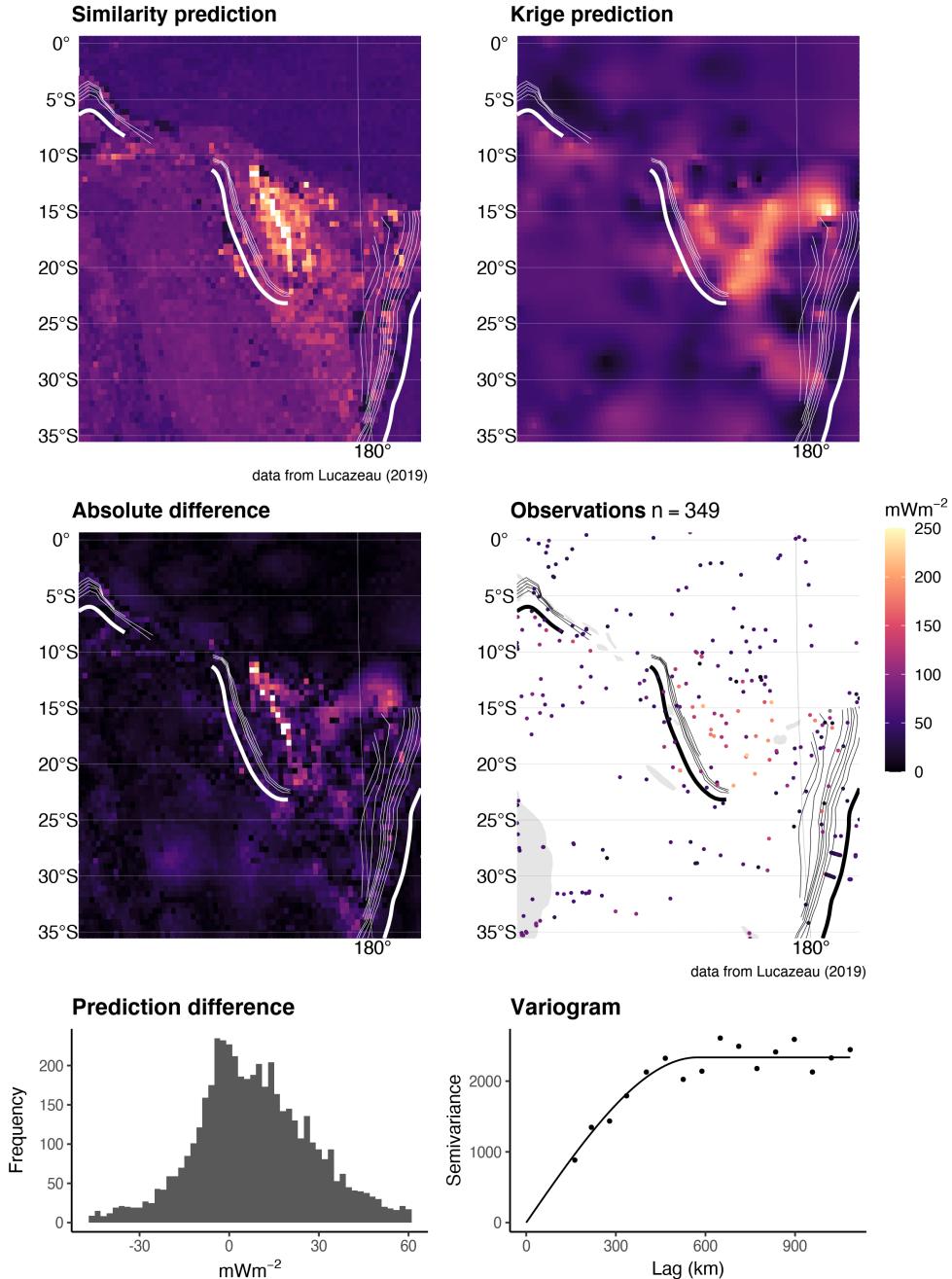


Figure 23: Similarity vs. Kriging predictions for Vanuatu.

617 **8.2 Kriging Optimization**

618 Achieving a useful Kriging results depends on one's choice of many Kriging parameters  
 619 ( $\Theta$ ). In this study, we investigate a set of parameters,  $\Theta$ :

$$\Theta = \{c, w, m, s, a, n, S\} \quad (10)$$

620 where  $c$  is the lag cutoff proportion,  $w$  is the lag window,  $m$  is the model type (sph  
 621 or exp),  $s$  is the sill,  $a$  is the effective range,  $n$  is the nugget, and  $S$  is the maximum dis-  
 622 tance for local Kriging. Only points within  $S$  from the prediction location are used for  
 623 Kriging. The lag cutoff is the maximum separation distance between pairs of points used  
 624 in the experimental variogram (i.e. the x-axis maximum limit) calculated as a fraction  
 625 of the overall maximum separation distance for all observations,  $Z(u)$ , in the domain,  
 626  $D$ . The lag window,  $w$ , shifts the lags where the variogram is evaluated by removing the  
 627 first  $n$  lags and adding  $n$  lags to the right side of the variogram. This is necessary to avoid  
 628 negative ranges,  $a$ , when fitting experimental variograms with anomalously high vari-  
 629 ances at small lag distances.

630 Our goal is to find  $\Theta$  such that our interpolation,  $f(x_i; \Theta)$ , gives the most useful  
 631 outcome—defined by minimizing a cost function,  $C(\Theta)$ —that represents the error be-  
 632 tween the set of real observations,  $Z(u_i)$  and predictions,  $\hat{Z}(u)$ . We define a cost func-  
 633 tion that simultaneously considers the misfit between the experimental and modelled var-  
 634 iogram and between the Kriging predictions and observed heat flow (after Z. Li et al.,  
 635 2018):

$$C(\Theta) = (1 - w)C_F(\Theta) + wC_I(\Theta) \quad (11)$$

636 where  $C_F(\Theta)$  is the root mean square error (RMSE) of the modelled variogram fit  
 637 calculated by WLS, and  $C_I(\Theta)$  is the RMSE of the Kriging result calculated by cross-  
 638 validation. The weight,  $w$ , is set to 0.5 in our study, which balances the effects of  $C_F(\Theta)$   
 639 and  $C_I(\Theta)$  on the cost function. The final expression to minimize becomes:

$$C(\Theta) = \frac{1-w}{\sigma_E} \sqrt{\frac{1}{N(h)} \sum_{k=1}^N w(h_k) [\hat{\gamma}(h_k) - \gamma(h_k; \Theta)]^2} + \frac{w}{\sigma_S} \sqrt{\frac{1}{M} \sum_{i=1}^M [Z(u_i) - \hat{Z}(u_i; \Theta)]^2} \quad (12)$$

where  $N(h)$  is the number of pairs of points used to calculate the experimental variogram,  $\hat{\gamma}(h_k)$ ,  $\sigma_E$  is the standard deviation of the experimental variogram,  $\hat{\gamma}(h)$ ,  $w(h_k)$  is the weight in WLS and defines the importance of the  $k$ th lag in the error estimate. We use  $w(h_k) = N_k/h_k^2$ .  $Z(u_i)$  and  $\hat{Z}(u_i; \Theta)$  are the measured and predicted values, respectively,  $\sigma_s$  is the standard deviation of the predicted values,  $\hat{Z}(u_i)$ , and  $M$  is the number of measurements in  $Z(u_i)$ . For  $C_I(\Theta)$  we use ten-fold cross-validation, which splits the dataset,  $|Z(u_i), \forall u_i \in D|$  into ten equal intervals and tests one interval against the remaining nine. This process is then repeated over all intervals so that the whole dataset has been cross-validated.

Minimization of  $C(\Theta)$  is achieved by a genetic algorithm that simulates biological natural selection by differential success (Goldberg, 1989). Our procedure is as follows:

1. Initiate fifty *chromosomes*,  $\xi$ , with random starting parameters defined within the search domain (Table 4)
2. Evaluate the fitness of each individual chromosome as  $-C(\Theta)$  for the entire population
3. Allow the population to exchange genetic information by sequentially performing genetic operations:
  - a. Selection: the top 5% fittest chromosomes survive each generation
  - b. Crossover: pairs of chromosomes have an 80% chance of exchanging genetic information
  - c. Mutation: there is a 10% chance for random genetic mutations
4. Evaluate the fitness of the new population
5. If the termination criterion is met, do step (6), otherwise continue to evolve by repeating steps (3) and (4)
6. Decode the best chromosome and build the optimal variogram

665 We use the general-purpose functions in the “R” package **GA** (Scrucca, 2013, 2017)  
 666 to perform each step in the above procedure.

Table 4: Parameters and ranges used in the optimization algorithm

Parameter	Search Domain	Units
Lag Cutoff (c)	[1/3, 1/15]	NA
Lag Window (w)	[1, 5]	NA
Model (m)	[Spherical, Exponential]	NA
Sill (s)	[1, 1000 $\sqrt{2}$ ]	$mWm^{-2}$
Effective Range (a)	[1, 1000]	km
Nugget (n)	[1, 1000 $\sqrt{2}$ ]	$mWm^{-2}$
Local Search (S)	[1, 1000]	km

667 **8.2.1 Genetic algorithm results**

668 **8.3 New Global Heat Flow Database References**

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