

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

Buchanan C. Kerswell ¹Matthew J. Kohn ¹

¹Department 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.,

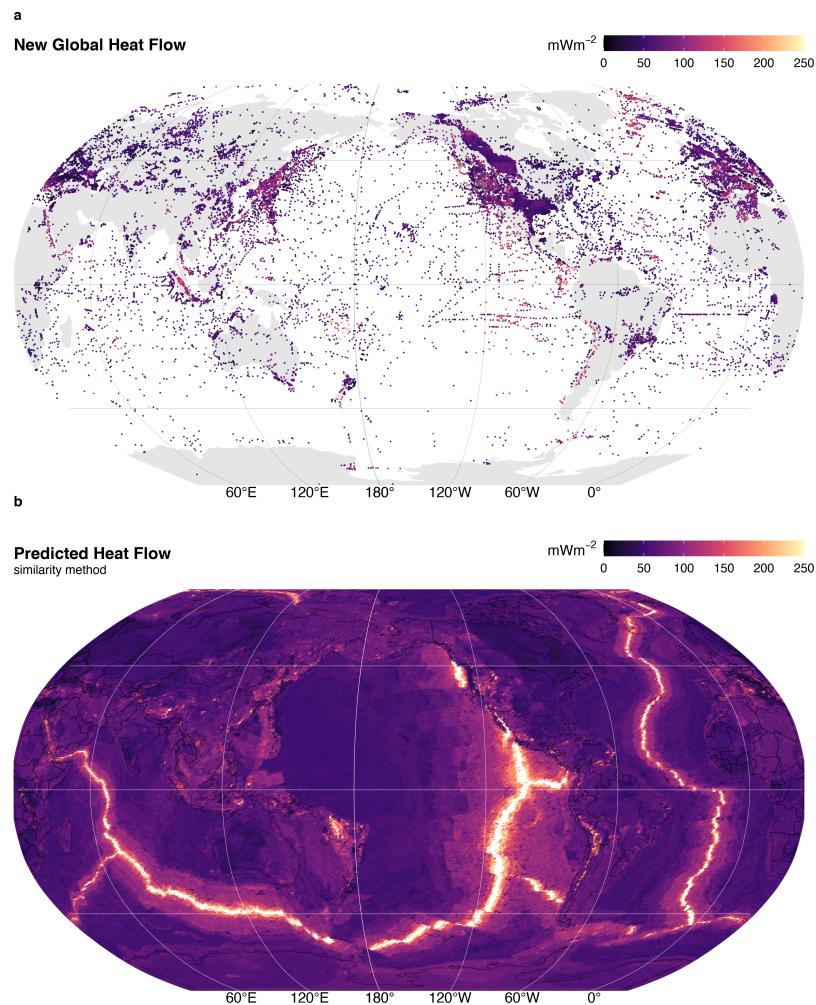


Figure 1: Global heat flow. (a) The NGHF database ($n = 69729$) and (b) interpolation by similarity method. Data from Luazeau (2019).

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 sampling heat flow along single
101 trench-perpendicular transects is an incomplete framework for hypothesis testing. Fur-
102 ther, inconsistent spatial continuity and heat flow patterns counter hypotheses of com-
103 mon thermal structure and geodynamics among subduction zones. We suggest future
104 research focus on generating high-quality interpolations and discuss considerations for
105 data acquisition priorities.

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. Lucaleau (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 vari-
 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):

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

where $N(h)$ is the number of pairs of points, $Z(u_i)$ and $Z(u_j)$, separated by a lag distance, $h = |u_i - u_j|$. We evaluate $\hat{\gamma}(h)$ at fifteen lag distances by binning the irregular spaced data with a bin width, δ , equal to a proportion of the maximum lag distance, c , divided by the number of lags used to evaluate the variogram. The lag cutoff parameter, c , is optimized by genetic algorithm (discussed below). The binwidth is then $\delta = \max(N(h))/(15c)$, and $N(h) \leftarrow N(h, \delta h) = \{i, j : |u_i - u_j| \in [h - \delta h, h + \delta h]\}$. In simple terms, Equation 2 represents the similarity, or dissimilarity, between pairs of observations in space. Equation 2 is adheres to the First Law of Geography and is derived from the theory of *regionalized variables* (Matheron, 1963, 2019), which formally defines a probabilistic framework for spatial interpolation of natural phenomena. It is important for the reader to understand the fundamental assumptions implicit in Equation 2 in order to understand the comparison of interpolation techniques discussed later. The basic assumptions used in our Kriging method are:

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

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

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

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 radioactive elements can be approximated by $q_s = q_b + \int A dz$, where q_b is a constant
 156 heat flux entering the bottom of the layer and A is the heat production within the
 157 layer with thickness z (Furlong & Chapman, 2013). If we have two samples, $Z(u_1) =$
 158 31 mW/m^2 and $Z(u_2) = 30.5 \text{ mW/m}^2$, their corresponding thicknesses would
 159 be $Z'(u_1) = 1000 \text{ m}$ and $Z'(u_2) = 500 \text{ m}$ for $A = 0.001 \text{ mW/m}^3$ and $q_b =$
 160 30 mW/m^2 . The variable, $Z(u)$, in this case is additive because the arithmetic mean
 161 of the samples is a good approximation of the average sedimentary layer thickness,
 162 $(Z(u_1) + Z(u_2))/2 = 750 \text{ m}$.
- 163
- 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 mW/m^2 , would correspond to plates with ages of $Z'(u_1) = 10 \text{ Ma}$, and $Z'(u_2) =$
 170 9 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:

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

197 The linear estimator must obey

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

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, λ_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:

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

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

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

214 2.3 Map Projection and Interpolation Grid

215 We interpolate onto the same 0.5°C x 0.5°C grid as F. Lucaleau (2019) so a di-
 216 rect difference could be calculated between our interpolation methods and F. Lucaleau
 217 (2019)'s. The NGHF and grid with predicted heat flow from F. Lucaleau (2019) were
 218 transformed into a Pacific-centered Robinson coordinate reference system (CRS) defined
 219 using the `proj` string (PROJ contributors, 2021):

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

222 All geographic operations, including Kriging and taking the difference with F. Lu-
 223 caleau (2019)'s heat flow predictions, are performed in the above CRS using the general-
 224 purpose functions in the "R" package `sf` (Pebesma, 2018). We define the Kriging do-
 225 main 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
grid for Kriging predictions so differences can be taken point-by-point at the exact same
locations. We provide the complete NGHF database (F. Lucaleau, 2019), filtered and
parsed NGHF database, heat flow interpolations (from F. Lucaleau, 2019, and this study),
and our code as supplementary information to support FAIR data policy (Wilkinson et
al., 2016). These materials can also be retrieved from the official repository at <https://doi.org/10.17605/OSF.IO/CA6ZU>.

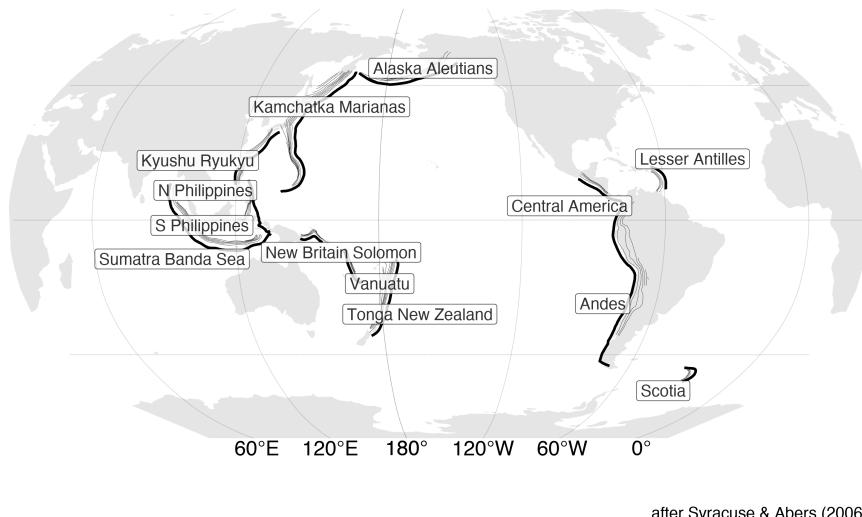
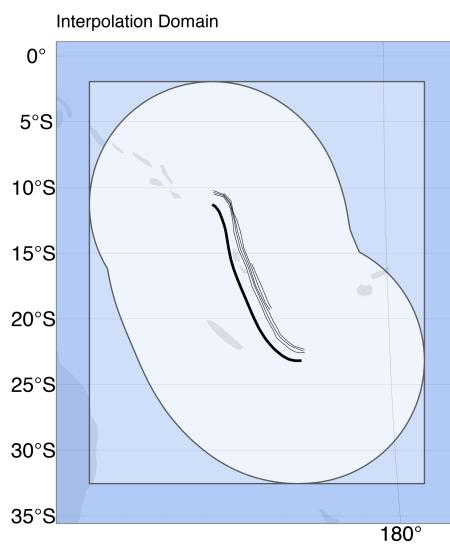
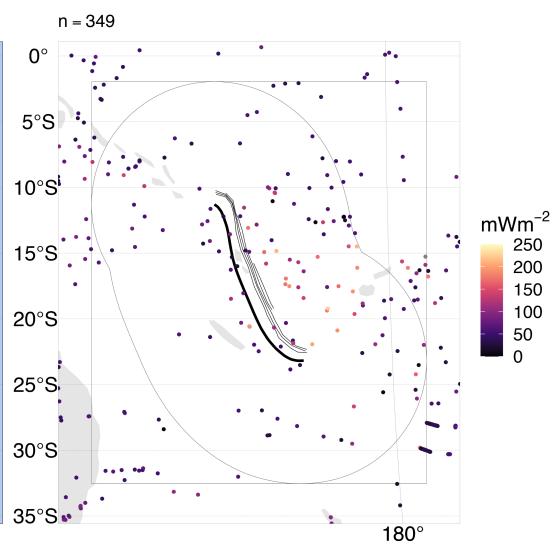
a Subduction Zone Segments**b Vanuatu****c Vanuatu**

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 Luceau (2019).

234 **3 Results**235 **3.1 Heat Flow Near Subduction Zone Segments**

236 Summary statistics for surface heat flow observations by subduction zone segment
 237 are given in Table 1 and Figure 3. Surface heat flow is median-centered around 65 mWm^{-2}
 238 and narrowly distributed for most subduction zone segments, excluding outliers, with
 239 inter-quartile ranges (IQR) median-centered around 43 mWm^{-2} . Alaska Aleutians is
 240 the exception with a higher median heat flow of 184 mWm^{-2} and broader range (IQR
 241 = 206 mW^{-2}). The whole distributions (including outliers) for all segments are strongly
 242 right-skewed with maximum heat flow values of several thousand of mWm^{-2} or more.
 243 Heat flow values above 250 mWm^{-2} are considered geothermal areas by F. Lucaleau
 244 (2019), which 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	184	206	233	344
Andes	5229	7	1710	45	50	87	91
Central America	5043	8	911	45	48	88	90
Kamchatka Marianas	3951	1	25200	70	48	116	574
Kyushu Ryukyu	3239	1	25200	72	45	125	633
Lesser Antilles	3536	13	1710	41	13	53	61
N Philippines	998	3	25200	71	35	191	1112
New Britain Solomon	180	3	174	64	42	69	30
S Philippines	1441	1	25200	71	43	156	924
Scotia	72	13	145	76	23	74	28
Sumatra Banda Sea	3033	1	1350	65	47	76	66
Tonga New Zealand	508	2	414	54	40	64	45
Vanuatu	349	2	283	54	40	64	44

245 **3.2 Variogram Models**

246 The optimal variogram models and associated errors are given in Table 2. Almost
 247 twice as many experimental variograms are fit with spherical models (10) compared to

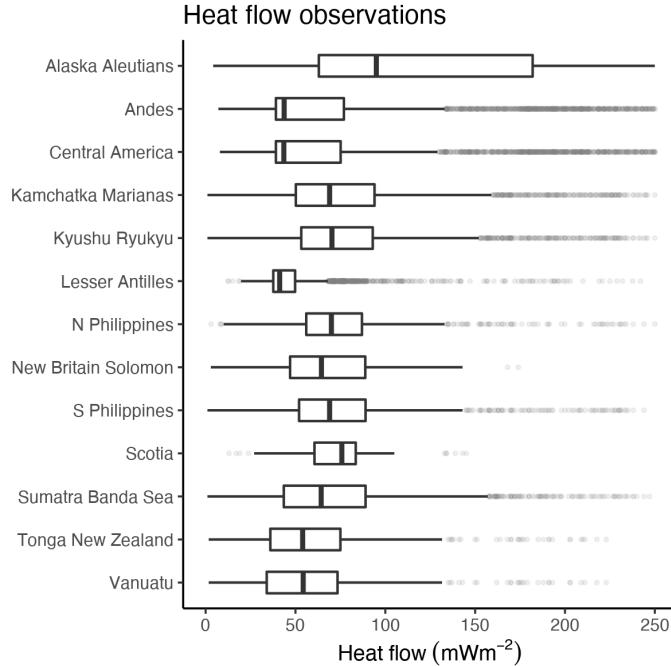


Figure 3: Distribution of heat flow observations. Heat flow near most segments is centered around $65 mW m^{-2}$ and highly skewed right (shadowy dot outliers). The skeweness likely represents sampling near geothermal systems, volcanic arcs, or spreading centers. Data from Lucaleau (2019).

248 exponential models (3). Variogram model sill vary substantially among the subduction
 249 zone segments between 9 and $1181 mW m^{-2}$. Variogram model ranges also vary substan-
 250 tially among segments from 4 to $1397 km$.

251 No apparent correlation exists between variogram model range and subduction zone
 252 segment length, number of heat flow observations, nor domain area (Figure 4). Most sub-
 253 duction zone segments show spatial dependence of a few hundred kilometers or less, ir-
 254 respective of the number of observations or segment size. The exceptions are Kyushu Ryukyu
 255 (range = $1397 km$) and Vanuatu (range = $573 km$), whose model variogram ranges are,
 256 perhaps, anomalously high.

Table 2: Optimal varigram models

Segment	Model	Sill [$mW m^{-2}$]	Range [km]
Alaska Aleutians	Sph	285	222
Andes	Sph	91	369
Central America	Sph	85	335

Segment	Model	Sill [mWm^{-2}]	Range [km]
Kamchatka Marianas	Exp	602	270
Kyushu Ryukyu	Sph	760	1397
Lesser Antilles	Sph	60	379
N Philippines	Sph	1181	238
New Britain Solomon	Exp	29	90
S Philippines	Sph	1011	415
Scotia	Exp	9	4
Sumatra Banda Sea	Sph	67	135
Tonga New Zealand	Sph	47	132
Vanuatu	Sph	48	573

257 3.3 Interpolation Comparison

258 Summary statistics for the interpolation differences are given in Table 3 and Fig-
 259 ure 5. Note that the difference is taken at the exact same locations for every prediction.
 260 Differences between the similarity method and Kriging are small for most segments with
 261 the exception of Central America, which shows a broader distribution of differences than
 262 the other segments. The median differences range from -9 to 8 mWm^{-2} with inter quar-
 263 tile ranges from 15 to 62 mWm^{-2} . Similar to the distribution of heat flow in these ar-
 264 eas, the minimum and maximum difference in predicted heat flow are extreme and rep-
 265 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	-552	2653	-2	20	3	71
Andes	-910	2338	2	36	13	73
Central America	-190	2731	8	62	44	146
Kamchatka Marianas	-2777	297	4	15	4	45
Kyushu Ryukyu	-2780	140	5	23	1	85
Lesser Antilles	-904	529	1	21	4	43
N Philippines	-2800	278	0	25	-5	94

Segment	Min	Max	Median	IQR	Mean	Sigma
New Britain Solomon	-81	236	2	22	5	20
S Philippines	-273	370	5	26	7	30
Scotia	-62	1001	-4	24	5	33
Sumatra Banda Sea	-308	386	0	20	2	20
Tonga New Zealand	-114	1695	-9	23	-2	30
Vanuatu	-166	1657	7	27	8	40

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

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

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

Variogram range correlations

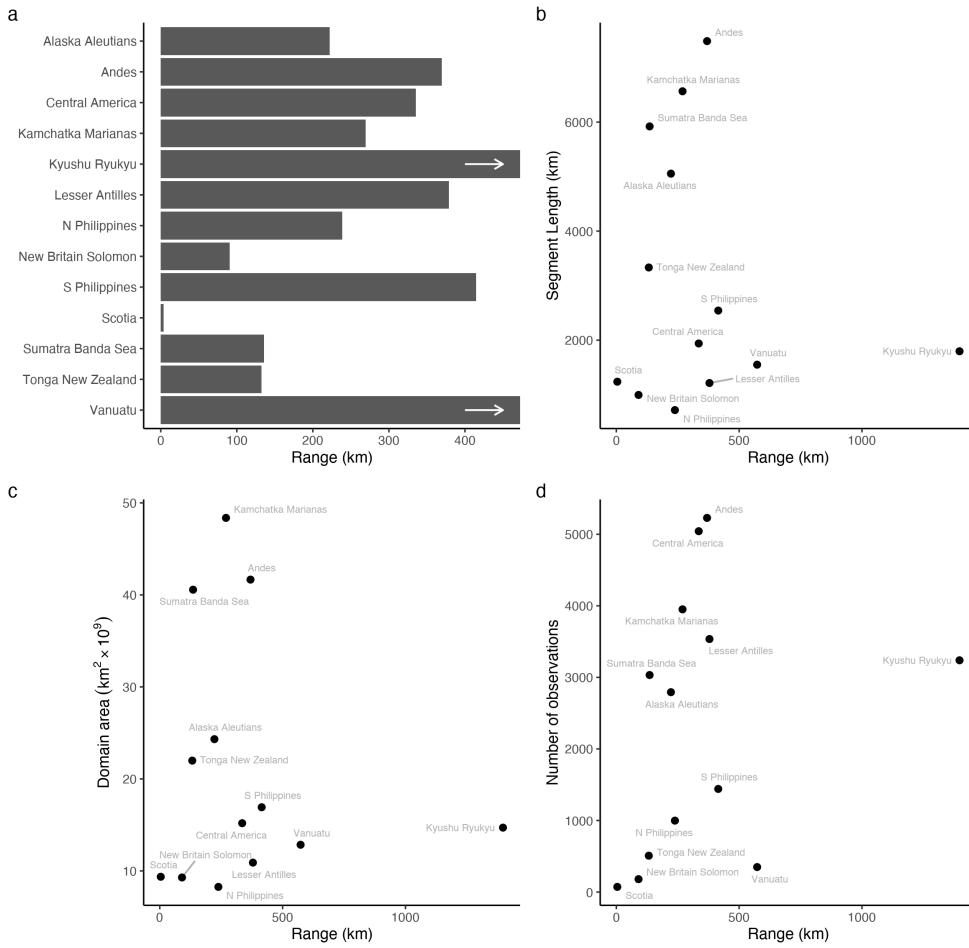


Figure 4: Summary of variogram model ranges and correlations with other features. (a) Variogram model ranges are variable, but generally below 400 km. Variogram model ranges show no correlation with segment length (b), number of heat flow observations (c), nor domain area (d). The spatial dependenc of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

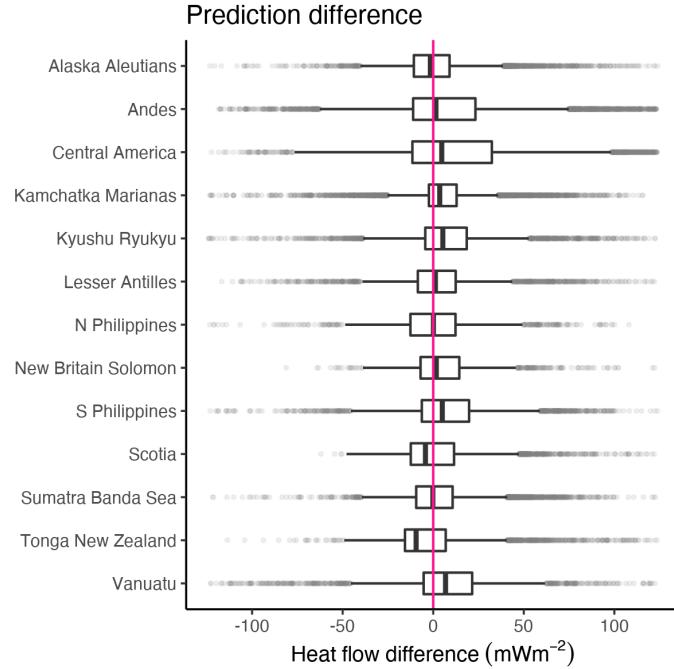


Figure 5: Point-by-point differences of predicted heat flow between similarity and Kriging interpolations (difference = similarity - Krige). The differences for most subduction zone segments are median-centered at or near-zero with IQRs from 15 to 62 mWm^{-2} . Outliers (shadowy dots) extend to extreme positive and negative differences.

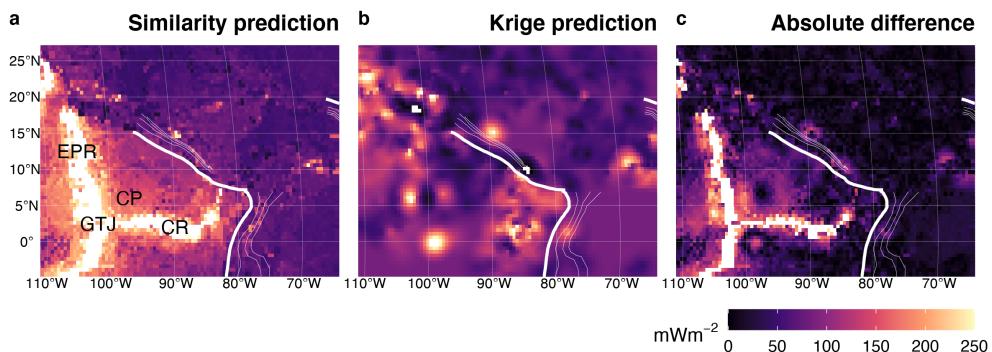


Figure 6: Similarity vs. Kriging predictions for Central America. The Galápagos triple junction (GTJ), East Pacific Rise (EPR), and Cocos Ridge (CR) are predicted by similarity (a), but not by Kriging (b). Note the moderate difference between predictions within the Cocos Plate (CP) where similarity predicts 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).

vational density and spatial coverage near the Lesser Antilles segment are sufficiently high 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.

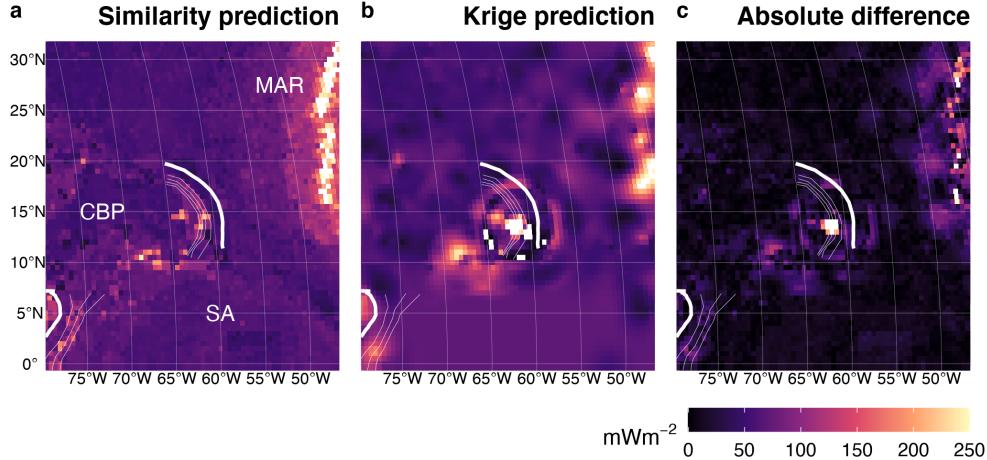


Figure 7: Similarity vs. Kriging predictions for the Lesser Antilles. The Mid-Atlantic Ridge (MAR) predicted by similarity (a) is also defined by Kriging (b) because of adequate observational density and spatial coverage near the spreading center. Good agreement between similarity and Kriging exist for 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).

Another example of good agreement between similarity and Kriging are interpolations near the Sumatra Banda Sea segment (Figures 8, 20). Note the textural and structural complexity predicted by similarity (Figure 8a) compared to the smooth featureless Kriging predictions (Figure 8b). 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 8c).

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 9a). Figure 9b 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,

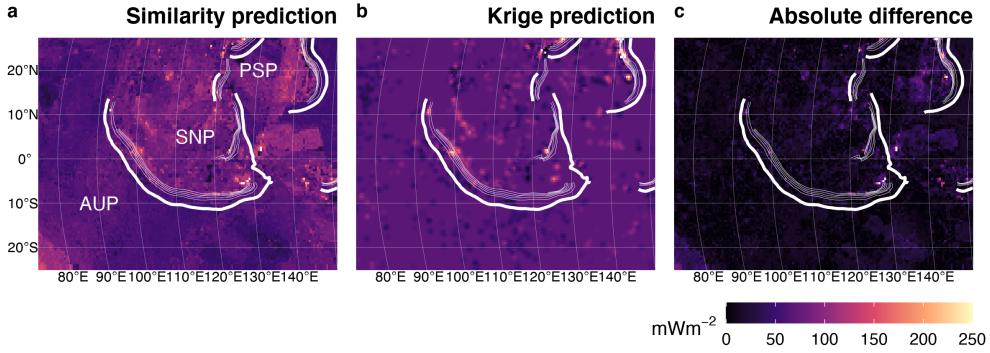


Figure 8: Similarity vs. Kriging predictions for Sumatra Banda Sea. Similarity predictions are texturally and structurally complex (a), while Kriging is smooth and featureless (b). Despite the textural and structural difference, the interpolations are similar, especially within the Sunda Plate (SNP), 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).

Table 2, Figure 21). Kriging predicts the expected (mean) heat flow value for the entire domain (Figure 9b), 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 9c). 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 10a). However, heat flow observations are sufficiently dense and continuous to partially resolve the short ridge segments and transform faults outlining the microplates between Vanuatu and the Tonga New Zealand segments by Kriging (Figure 10b). The differences (Figure 10c) are difficult to interpret because of the somewhat random discordance between interpolation methods.

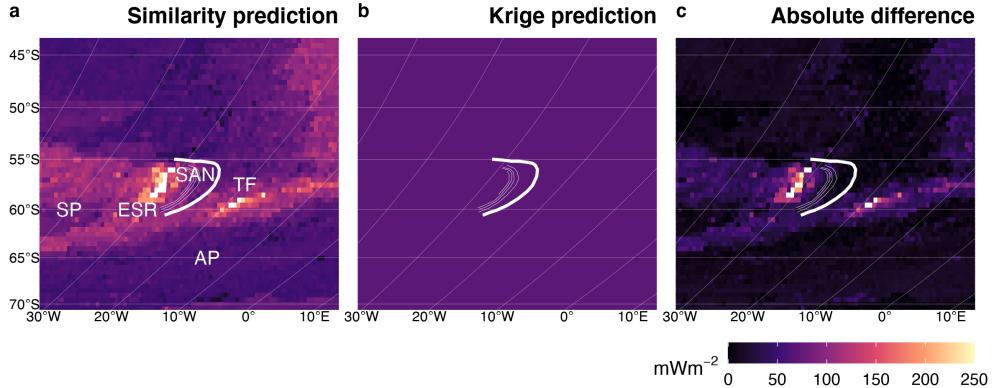


Figure 9: Similarity vs. Kriging predictions for Scotia. (a) Similarity predicts high heat flow for two tectonic features, the East Scotia Ridge (ESR) and a transform fault (TF) separating the Scotia and Sandwich Plates (SP, SAN) from the Antarctic Plate (AP). Kriging (b) is featureless because of incredibly 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 Lucaleau (2019).

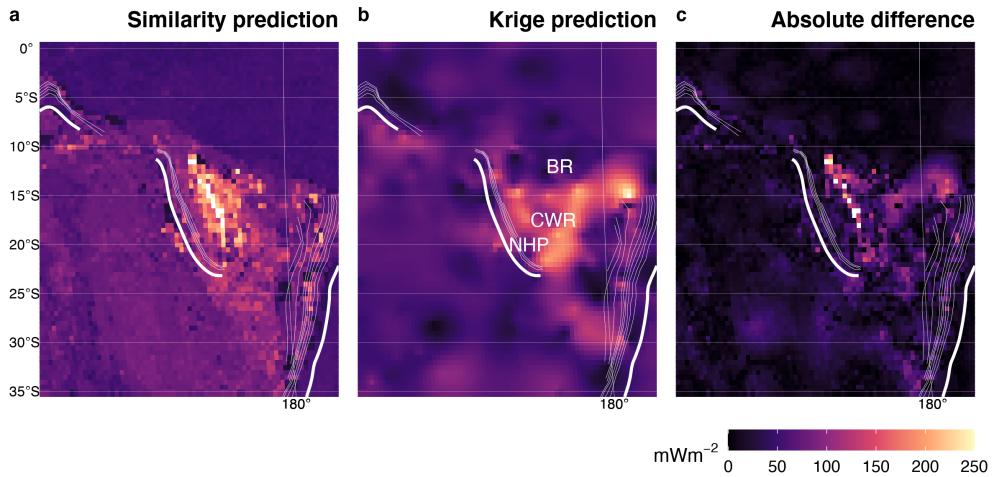


Figure 10: Similarity vs. Kriging predictions for Vanuatu. (a) Similarity resolved the spreading center separating the New Hebrides Plate (NHP) from the Balmoral Reef (BR) and Conway Reef (CR) microplates. Sufficient heat flow observations allow Kriging to resolve additional ridge segments and transform 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 Lucaleau (2019).

322 **4 Discussion**

323 **4.1 The First and Third Laws of Geography**

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

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

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

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

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

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

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

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

386 **4.2 Hypothesis Testing**

387 Testing hypotheses relating to subduction dynamics require sampling of heat flow
388 in order to apply statistical models. Sampling in previous work commonly uses a three-
389 part strategy: 1) draw a cross-section line perpendicular to the trench, 2) draw a rect-
390 angle with arbitrary width bisected by the section line, 3) gather all heat flow observa-
391 tions within the rectangle and project them onto the section line (e.g., Currie et al., 2004;
392 Currie & Hyndman, 2006; Roy D. Hyndman et al., 2005; Wada & Wang, 2009). This sam-
393 pling strategy is simple and most effective if measurements along section lines are equally
394 spaced with high spatial density. Observations along straight transects perpendicular to
395 trenches, however, are rare in the NGHF except for a few studies e.g. near the Lesser An-
396 tilles and Sumatra Banda Sea segments, 16, Figure 20, (F. Luazeau, 2019). There are
397 additional limitations to this method, including: 1) the method increasingly violates the
398 First Law as the size of the sampling rectangle increases—projecting more disparate points
399 onto the section line—and 2) sampling must be repeated many times along strike to fully
400 characterize the spatial distribution of heat flow near subduction zone segments. Despite
401 these limitations, previous work use single transects to characterize whole subduction
402 zones, which are then compared to make broad claims about global subduction dynam-
403 ics (e.g., Currie et al., 2004; Currie & Hyndman, 2006; Roy D. Hyndman et al., 2005;
404 Kerswell et al., 2020; Wada & Wang, 2009).

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

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

419 **4.3 Heat Flow Sampling Strategies**

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

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

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

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

443 Surveying heat flow is temporally, energetically, and monetarily expensive. We sug-
 444 gest prioritizing small segments like Scotia, the Lesser Antilles, and New Britain Solomon
 445 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.

475 5 Conclusions

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

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

493 6 Open Research

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

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609 **8 Appendix**

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

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

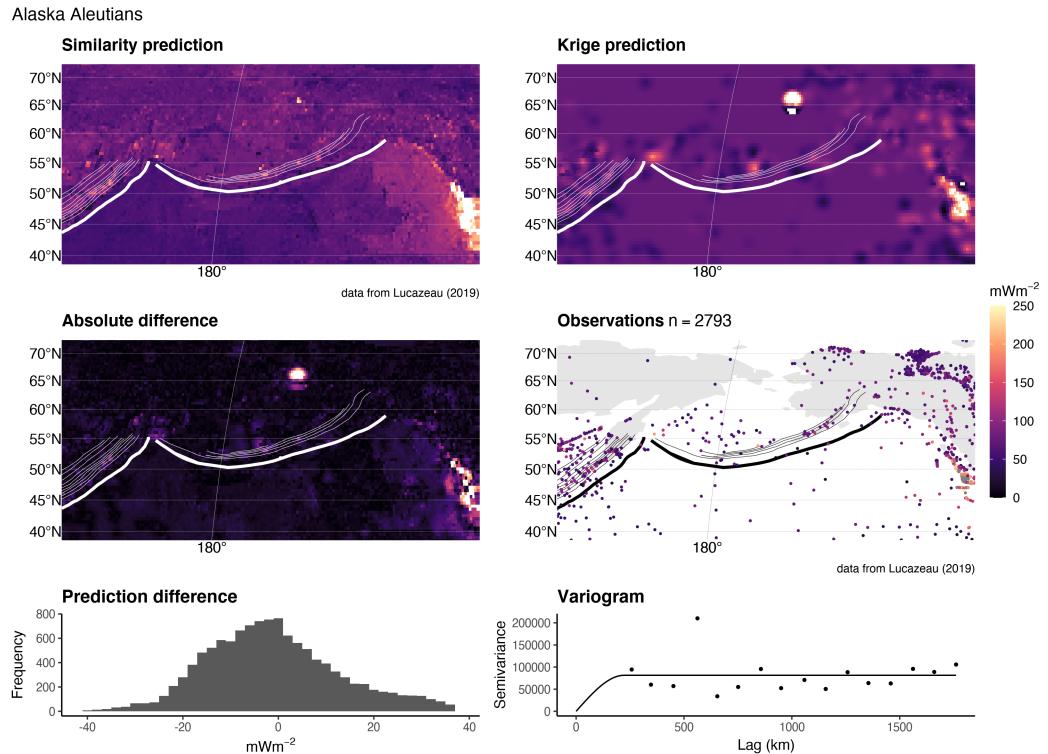


Figure 11: Similarity vs. Kriging predictions for Alaska Aleutians.

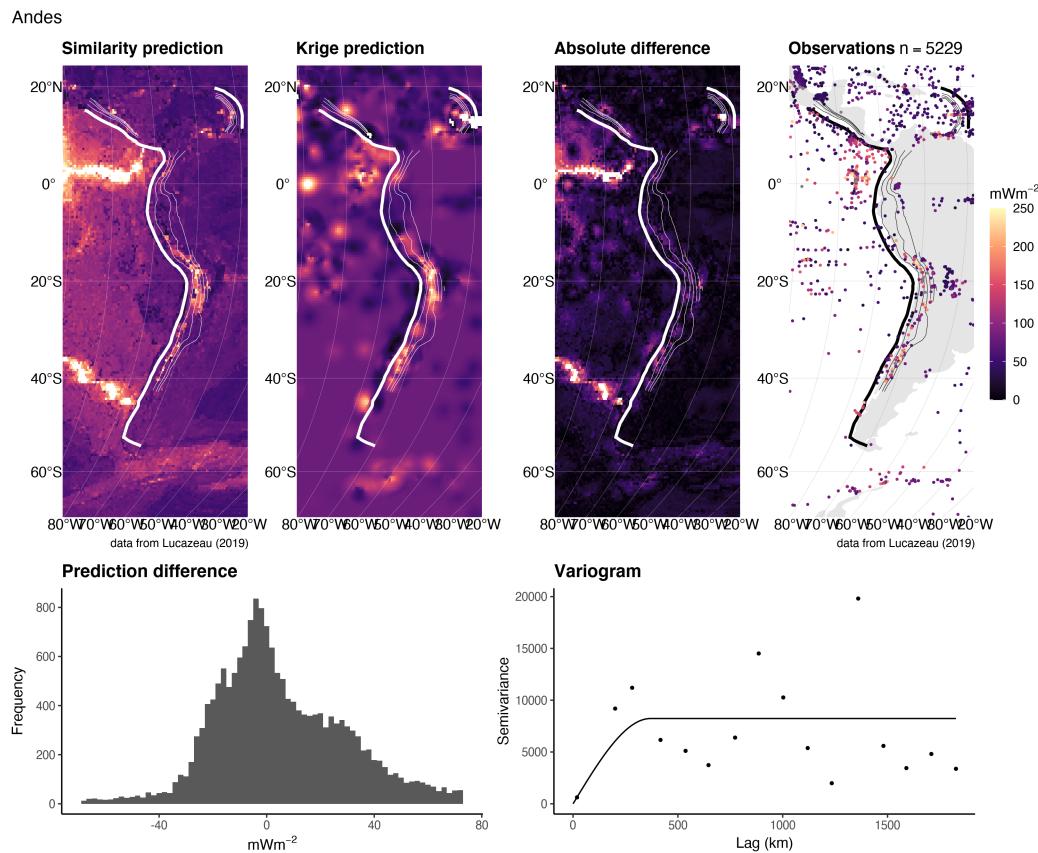


Figure 12: Similarity vs. Kriging predictions for the Andes.

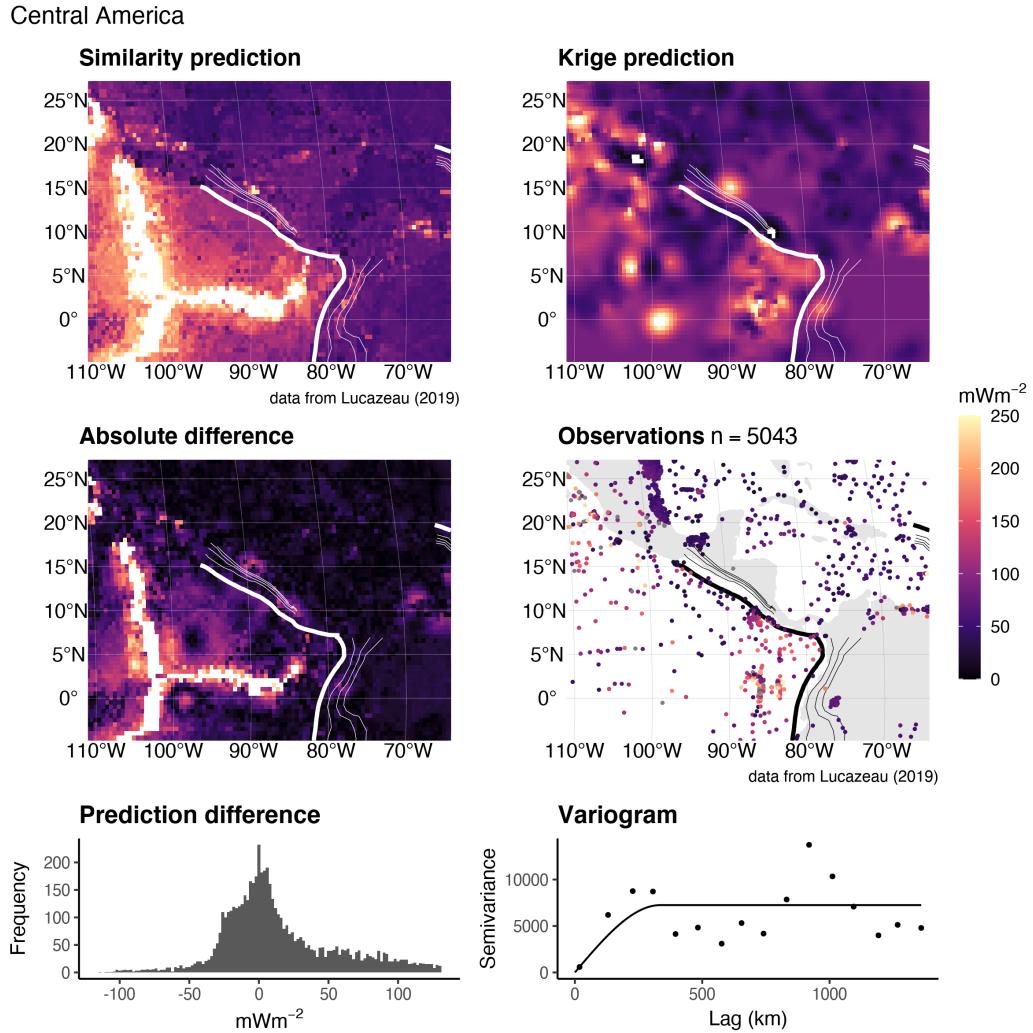


Figure 13: Similarity vs. Kriging predictions for Central America.

Kamchatka Marianas

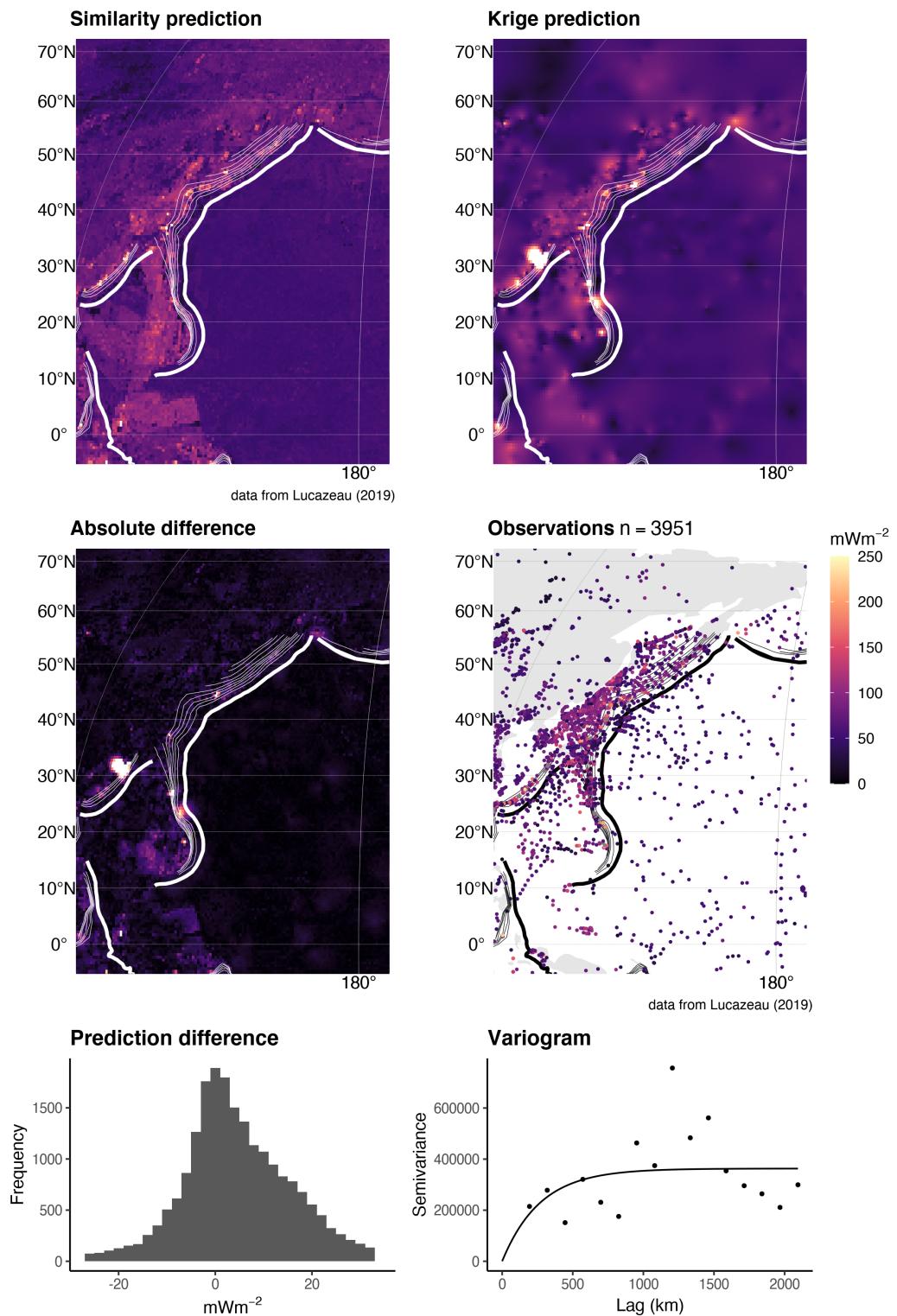


Figure 14: Similarity vs. Kriging predictions for Kamchatka Marianas.

Kyushu Ryukyu

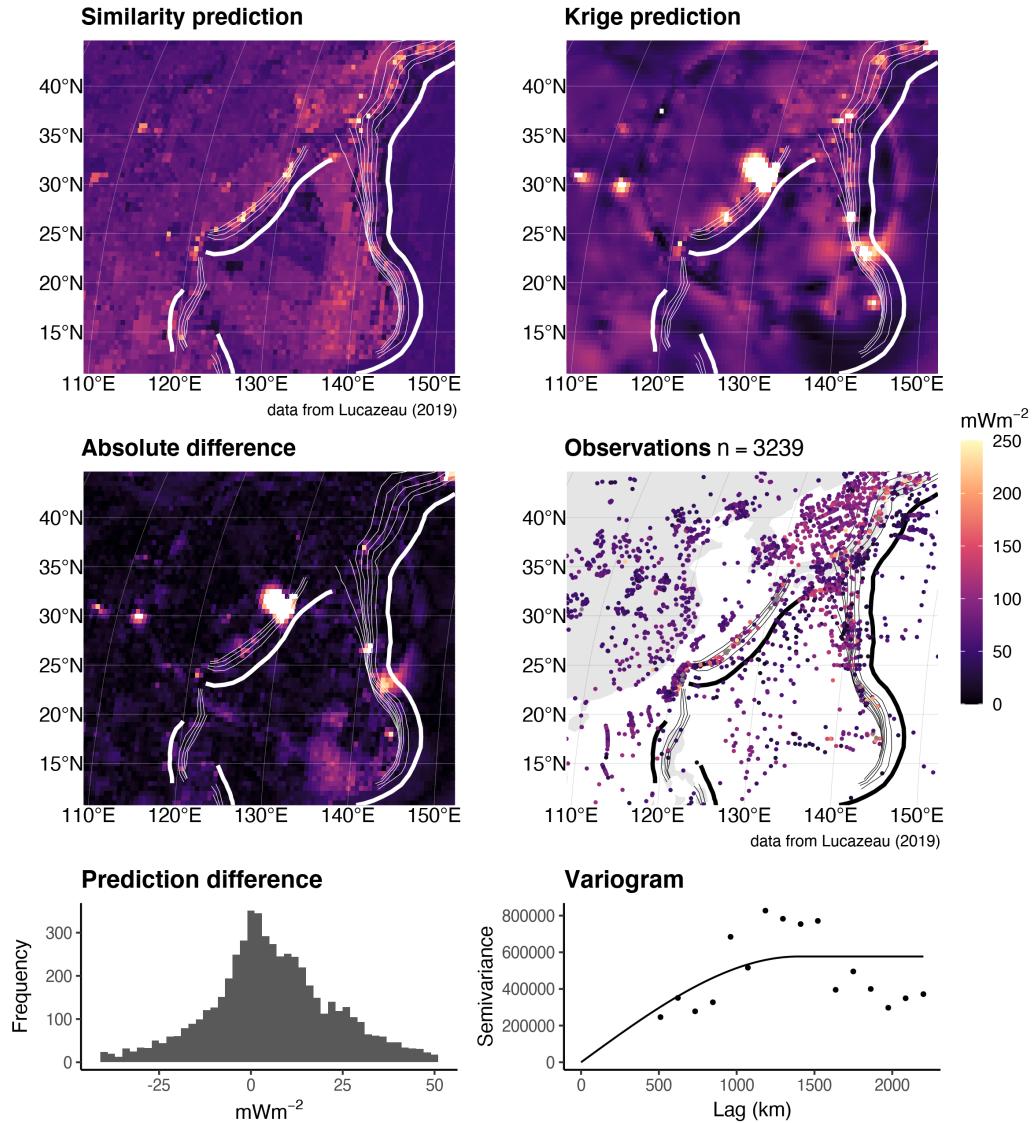


Figure 15: Similarity vs. Kriging predictions for Kyushu Ryukyu.

Lesser Antilles

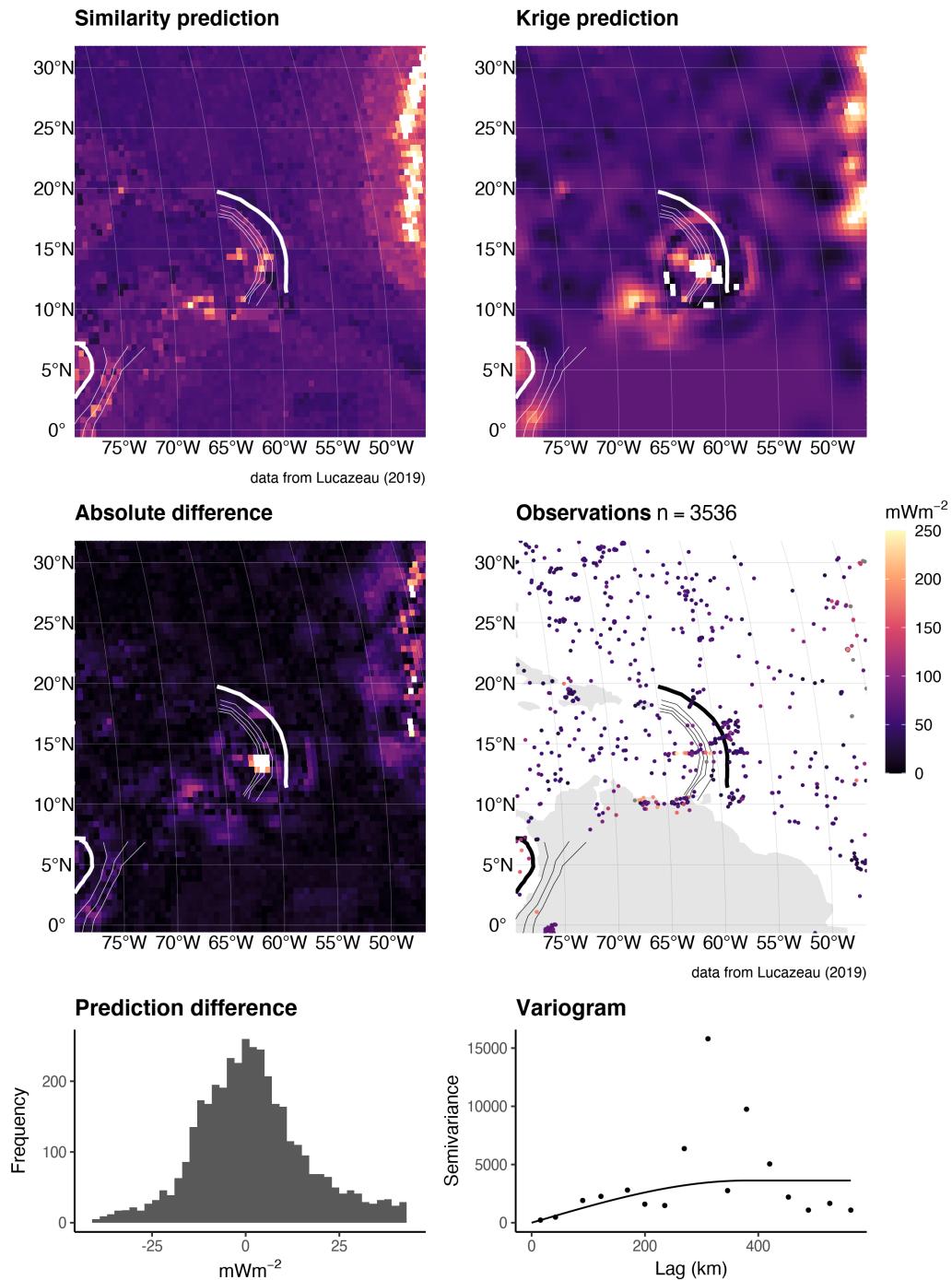


Figure 16: Similarity vs. Kriging predictions for the Lesser Antilles.

N Philippines

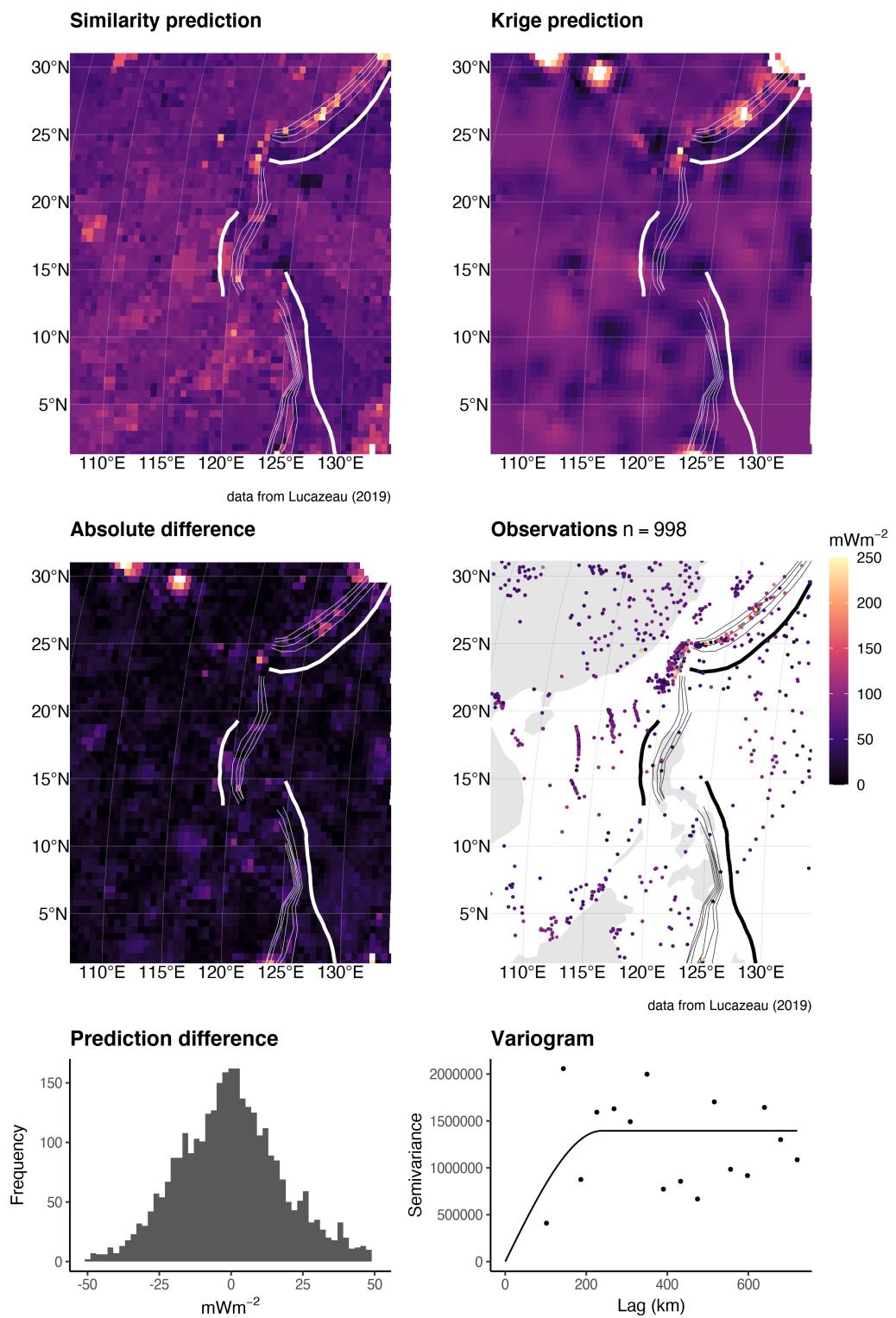


Figure 17: Similarity vs. Kriging predictions for N. Philippines.

New Britain Solomon

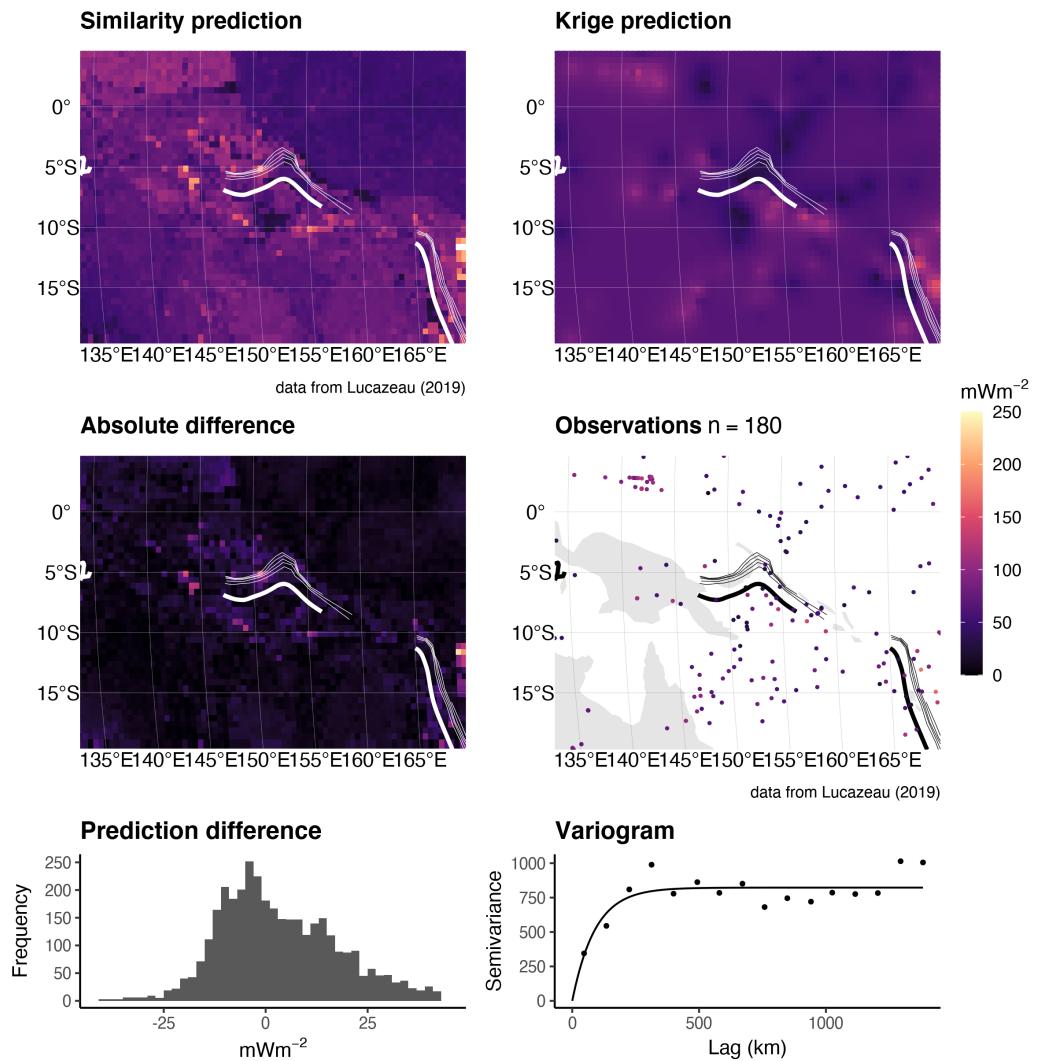


Figure 18: Similarity vs. Kriging predictions for New Britain Solomon.

S Philippines

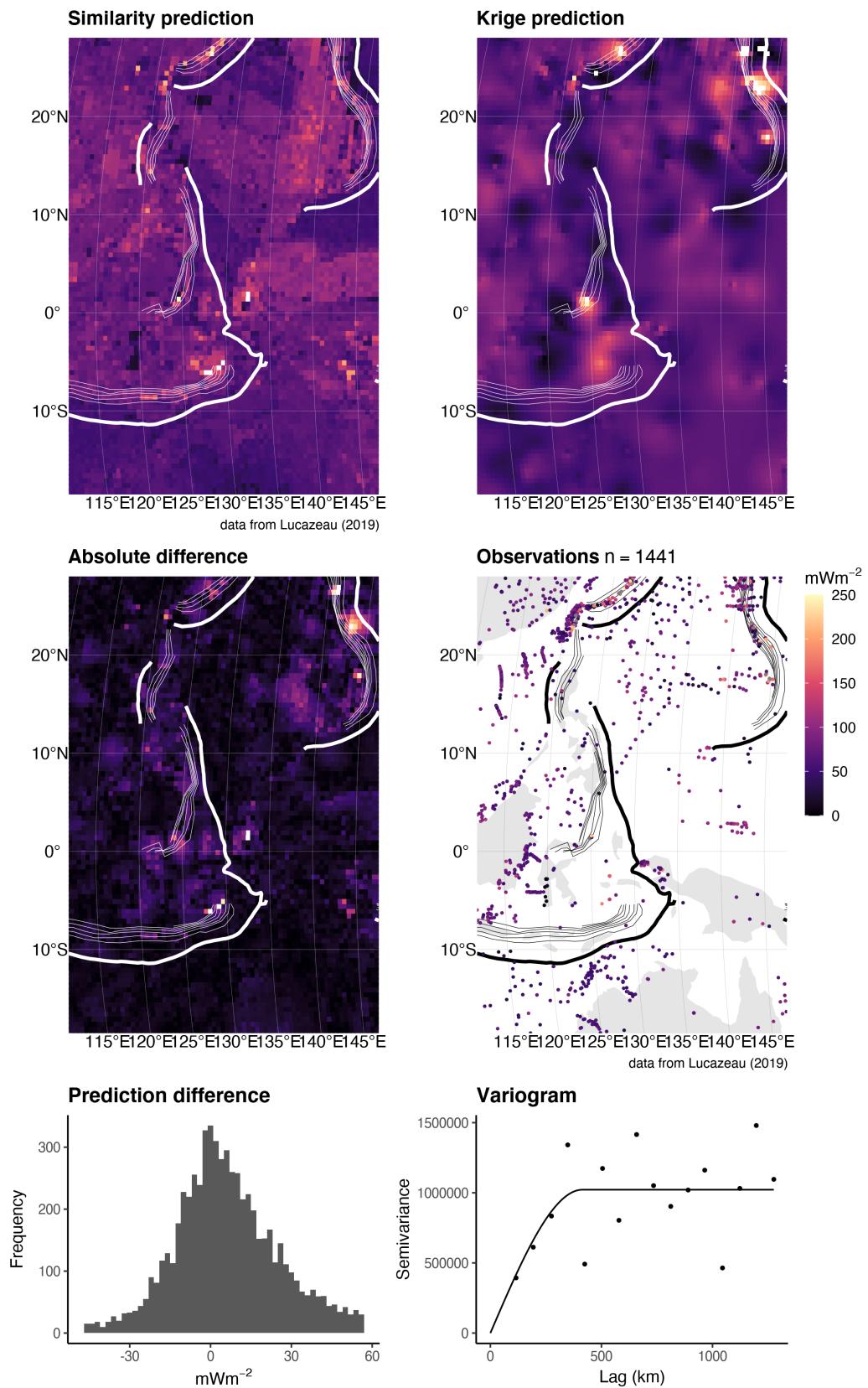


Figure 19: Similarity vs. Kriging predictions for S. Philippines.

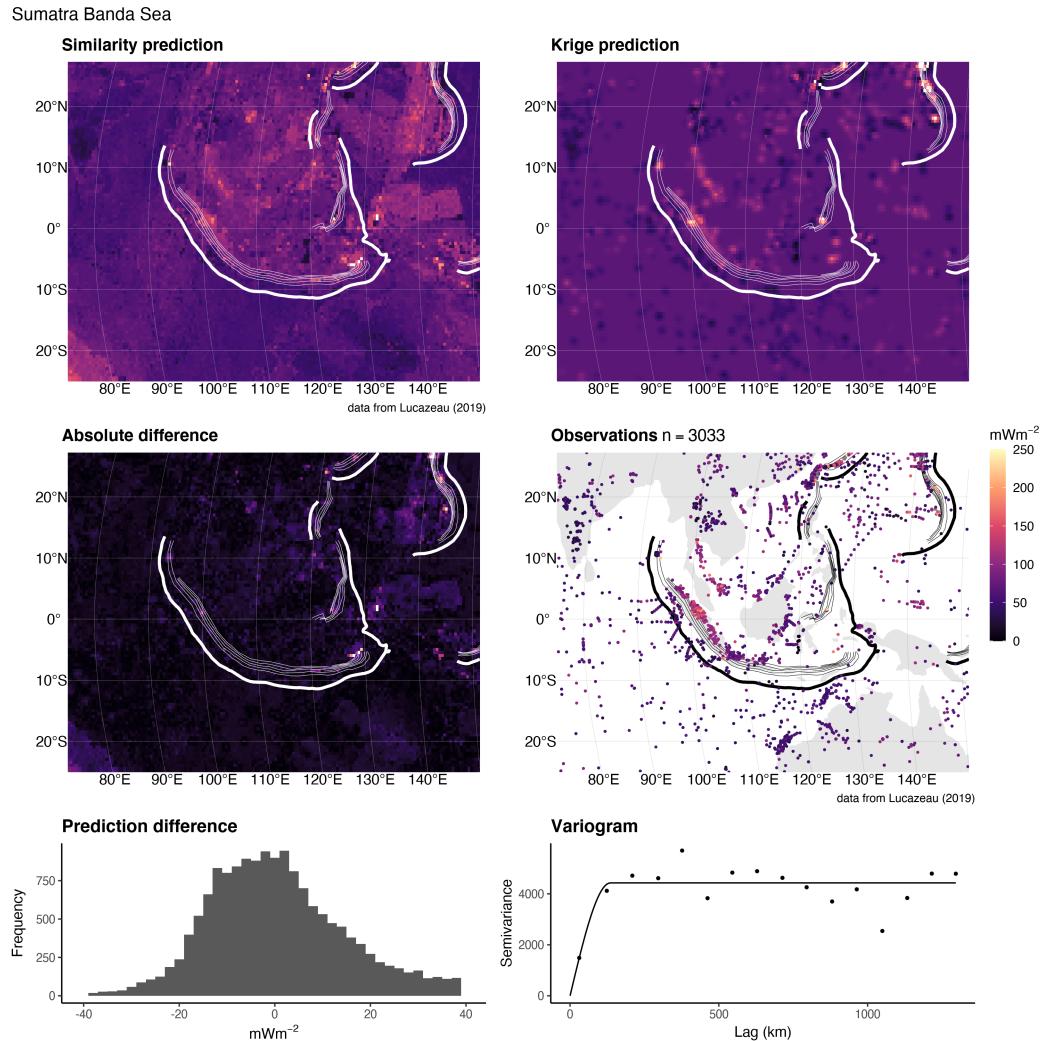


Figure 20: Similarity vs. Kriging predictions for Sumatra Banda Sea.

Scotia

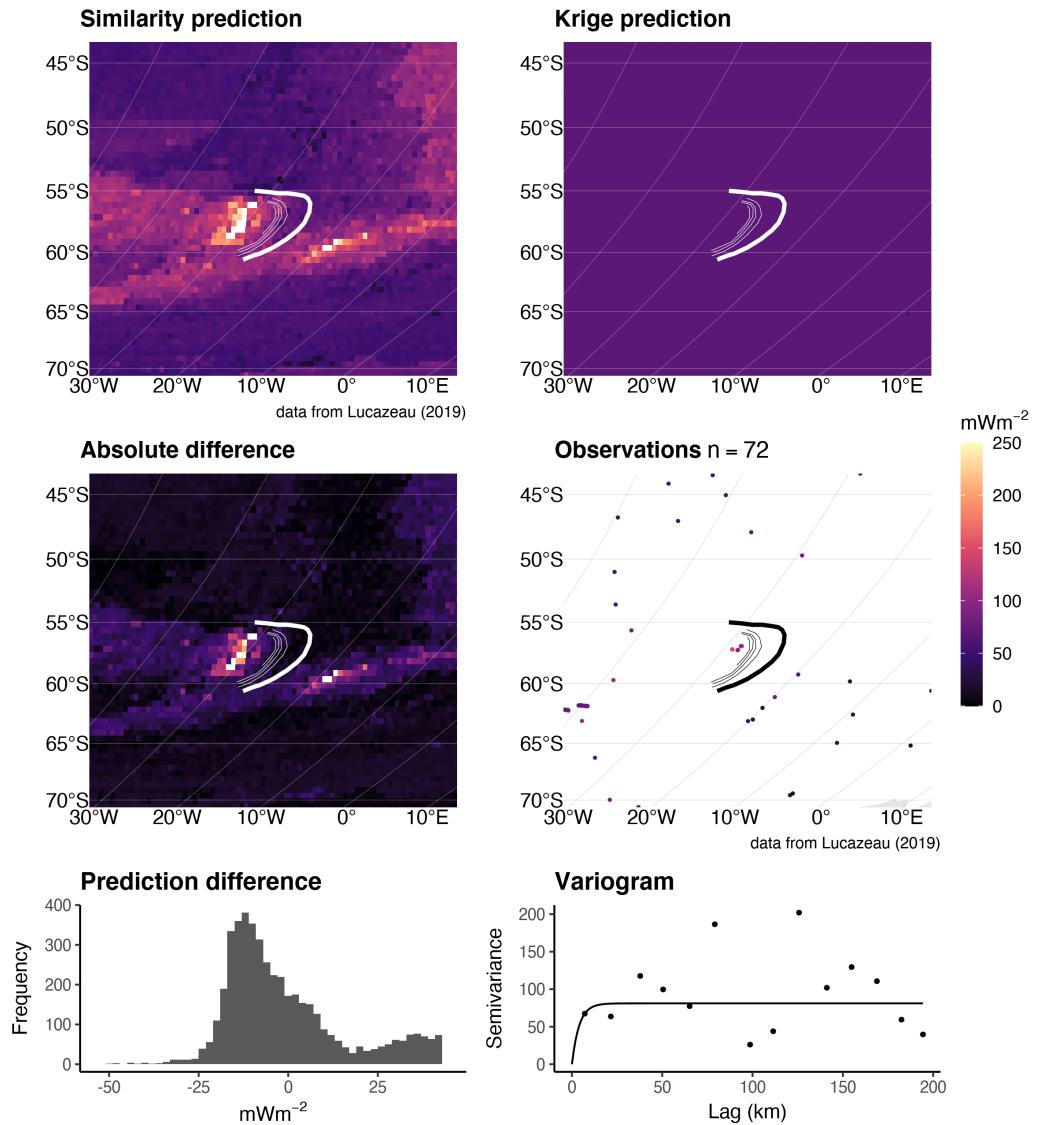


Figure 21: Similarity vs. Kriging predictions for Scotia.

Tonga New Zealand

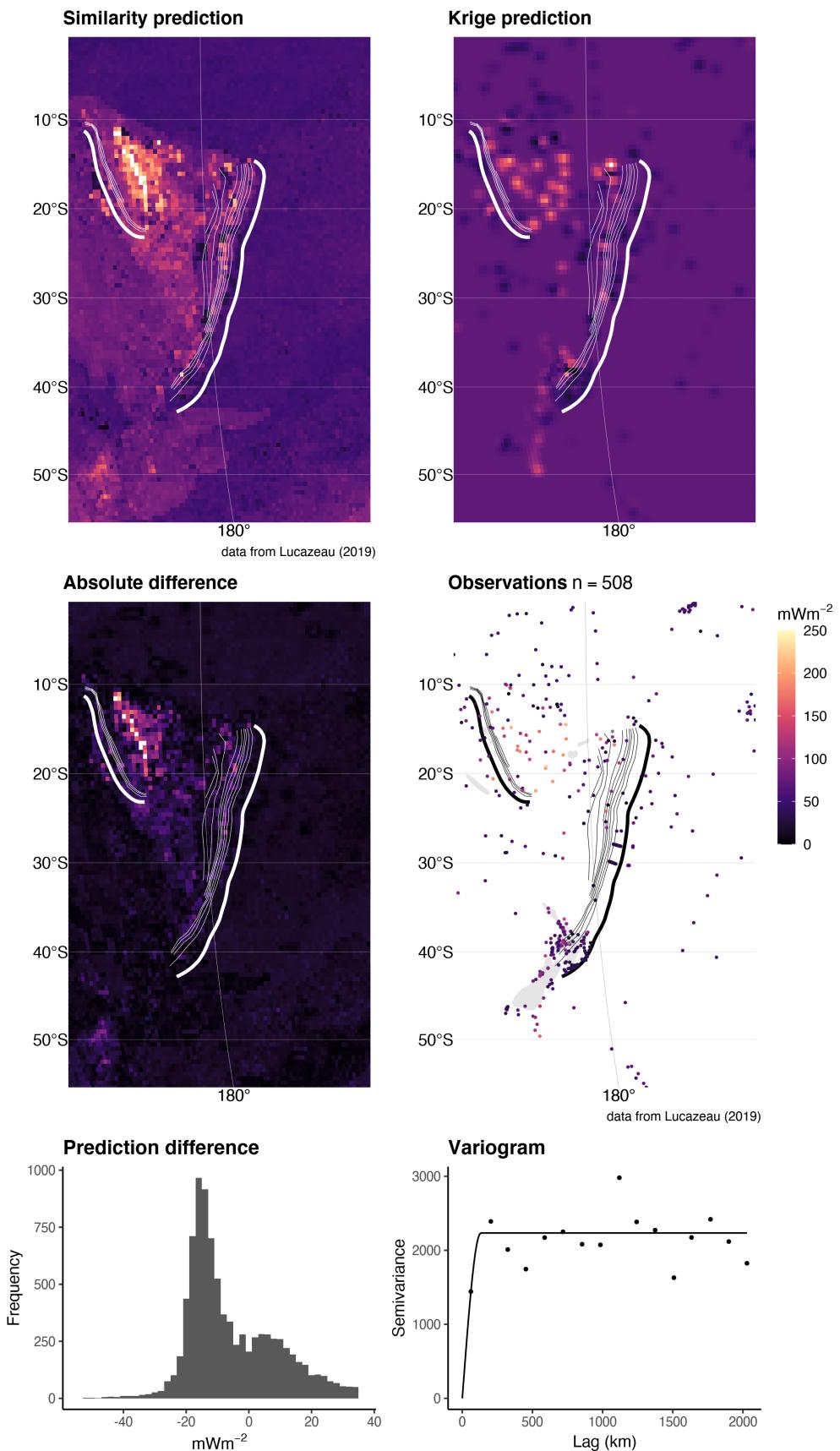


Figure 22: Similarity vs. Kriging predictions for Tonga New Zealand.

Vanuatu

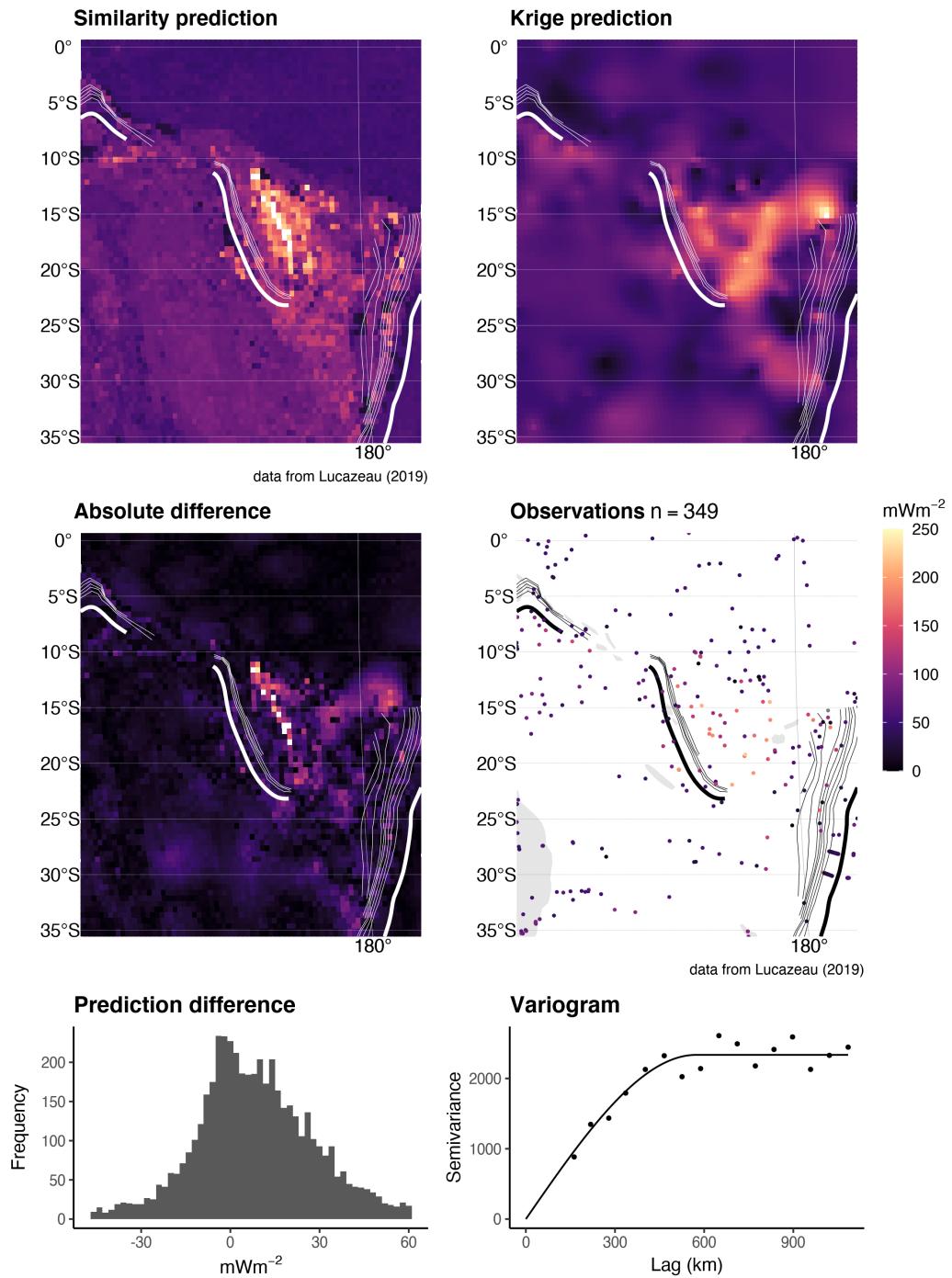


Figure 23: Similarity vs. Kriging predictions for Vanuatu.

616 **8.2 Kriging optimization by genetic algorithm**

617 Achieving a useful Kriging results depends on one's choice of many Kriging parameters (Θ). In this study, we investigate a set of parameters, Θ:

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

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

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

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

635 where $C_F(\Theta)$ is the root mean square error (RMSE) of the modelled variogram fit
 636 calculated by WLS, and $C_I(\Theta)$ is the RMSE of the Kriging result calculated by cross-
 637 validation. The weight, w , is set to 0.5 in our study, which balances the effects of $C_F(\Theta)$
 638 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, $\hat{\gamma}(h_k)$, σ_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, σ_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*, ξ , 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

664 We use the general-purpose functions in the “R” package **GA** (Scrucca, 2013, 2017)
 665 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, 10000]	km

666 **8.3 Heat flow observations and predictions optimized by genetic algo-**
 667 **rithm**

668 The optimal variogram models and associated cost $C(\Theta)$ are given in Table 5. Fig-
 669 ure 24 shows comparisons between the variograms fit by ordinary least squares (default,
 670 Pebesma, 2004) and genetic algorithm (after Z. Li et al., 2018). Table 6 and Figure 25
 671 show the differences between Kriging predictions optimized by genetic algorithm and sim-
 672 ilarity prediction of F. Lucazeau (2019). Finally, Figures ??, ??, ??, ??, ??, ??, 26, 27,
 673 28, ??, 29, 30, 31 show the heat flow observations and Kriging predictions optimized by
 674 genetic algorithm for all subduction zone segments.

Table 5: Optimal varigram parameters by genetic algorithm

Segment	c	w	m	s [mWm^{-2}]	a [km]	n [mWm^{-2}]	S [km]	Cost
N Philippines	7	3.2	Exp	838	326	919	6170	0.608
New Britain Solomon	6	2.7	Sph	976	702	1060	31	0.182
S Philippines	9	3.4	Exp	986	141	987	5566	0.553
Scotia	9	3.3	Exp	1026	571	306	129	0.192
Tonga New Zealand	9	2.8	Sph	977	517	953	236	0.422
Vanuatu	5	3.2	Sph	1045	727	1048	37	0.271

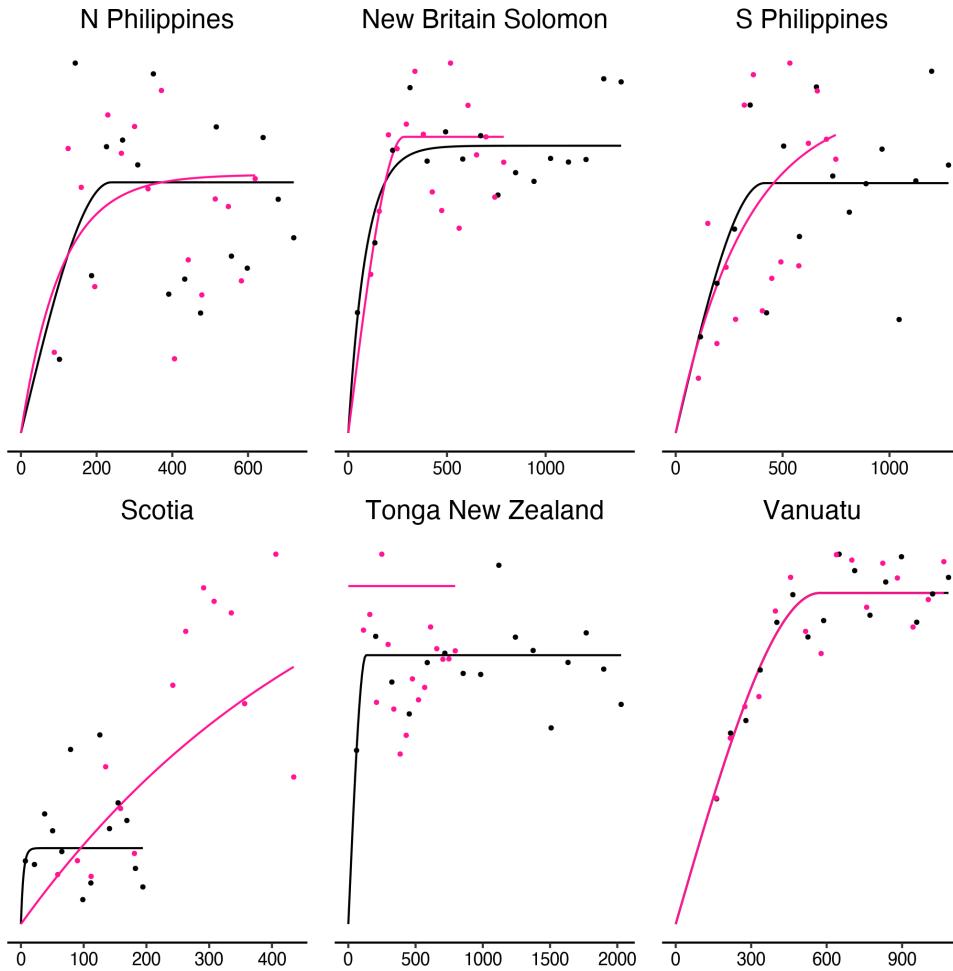


Figure 24: Comparison between variograms fit by ordinary least squares (black) and genetic algorithm (pink). The black variogram models are adjusted until ordinary least squares regression gives a tolerable fit. Pink variogram models are fit without human intervention.

Table 6: Predicted heat flow (mWm^{-2}) differences (GA)

Segment	Min	Max	Median	IQR	Mean	Sigma
N Philippines	-2764	275	1	22	-4	86
New Britain Solomon	-91	238	2	22	6	21
S Philippines	-270	357	6	25	7	28
Scotia	-93	1012	11	32	13	33
Tonga New Zealand	-58	1706	-4	23	5	31
Vanuatu	-166	1656	7	27	8	40

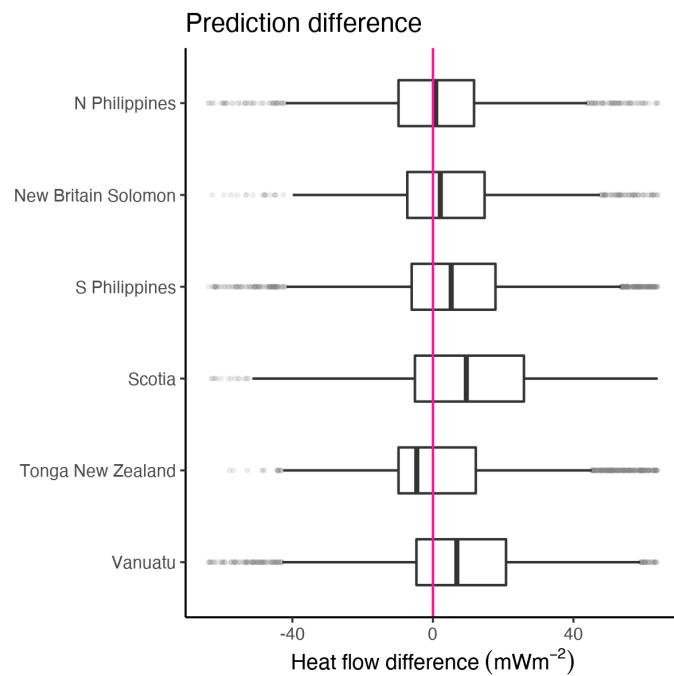


Figure 25: Point-by-point differences of predicted heat flow between similarity and Kriging interpolations (difference = similarity - Krige). Kriging results were optimized by a genetic algorithm. The differences for most subduction zone segments are median-centered at or near-zero with IQRs from 16 to 62. Outliers (shadowy dots) extend to extreme positive and negative differences.

N Philippines

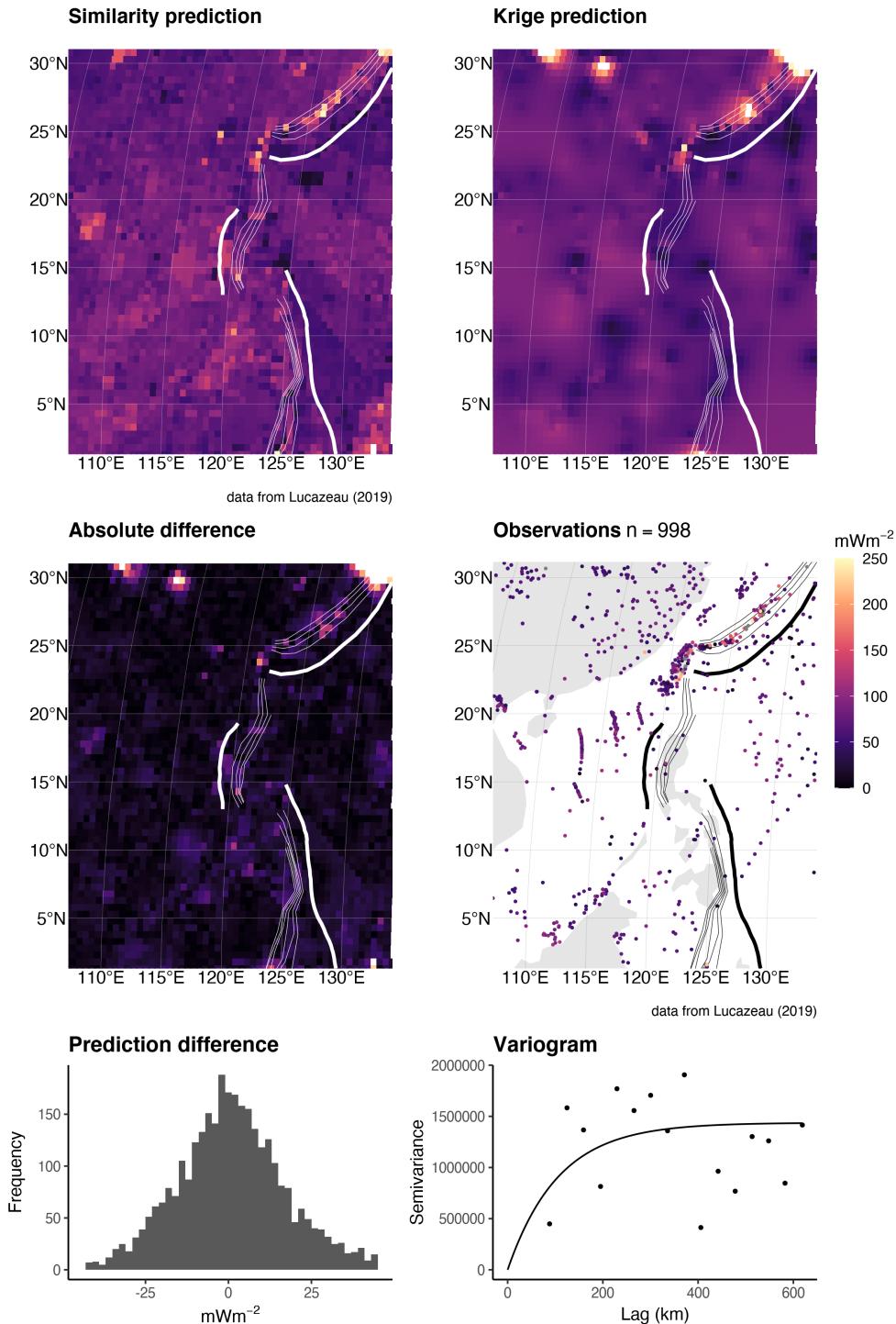


Figure 26: Similarity vs. Kriging predictions for N. Philippines. Kriging predictions are optimized by genetic algorithm.

New Britain Solomon

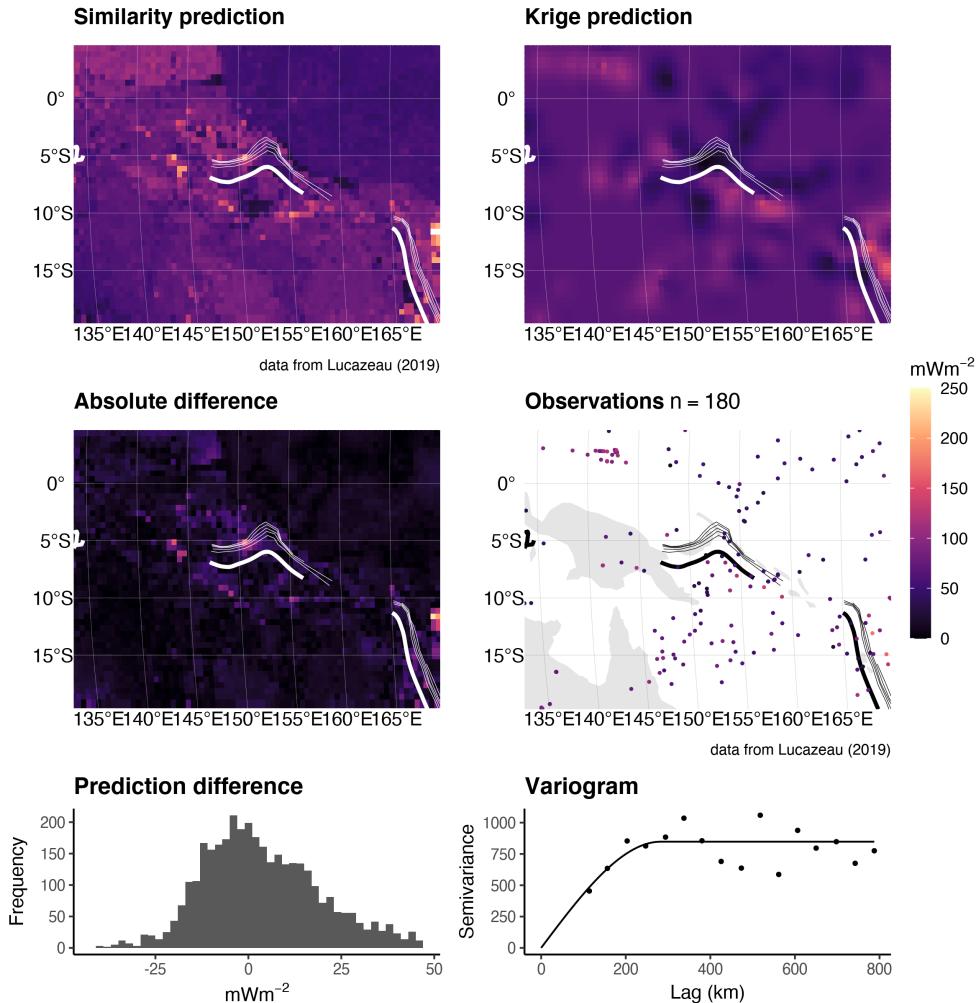


Figure 27: Similarity vs. Kriging predictions for New Britain Solomon. Kriging predictions are optimized by genetic algorithm.

S Philippines

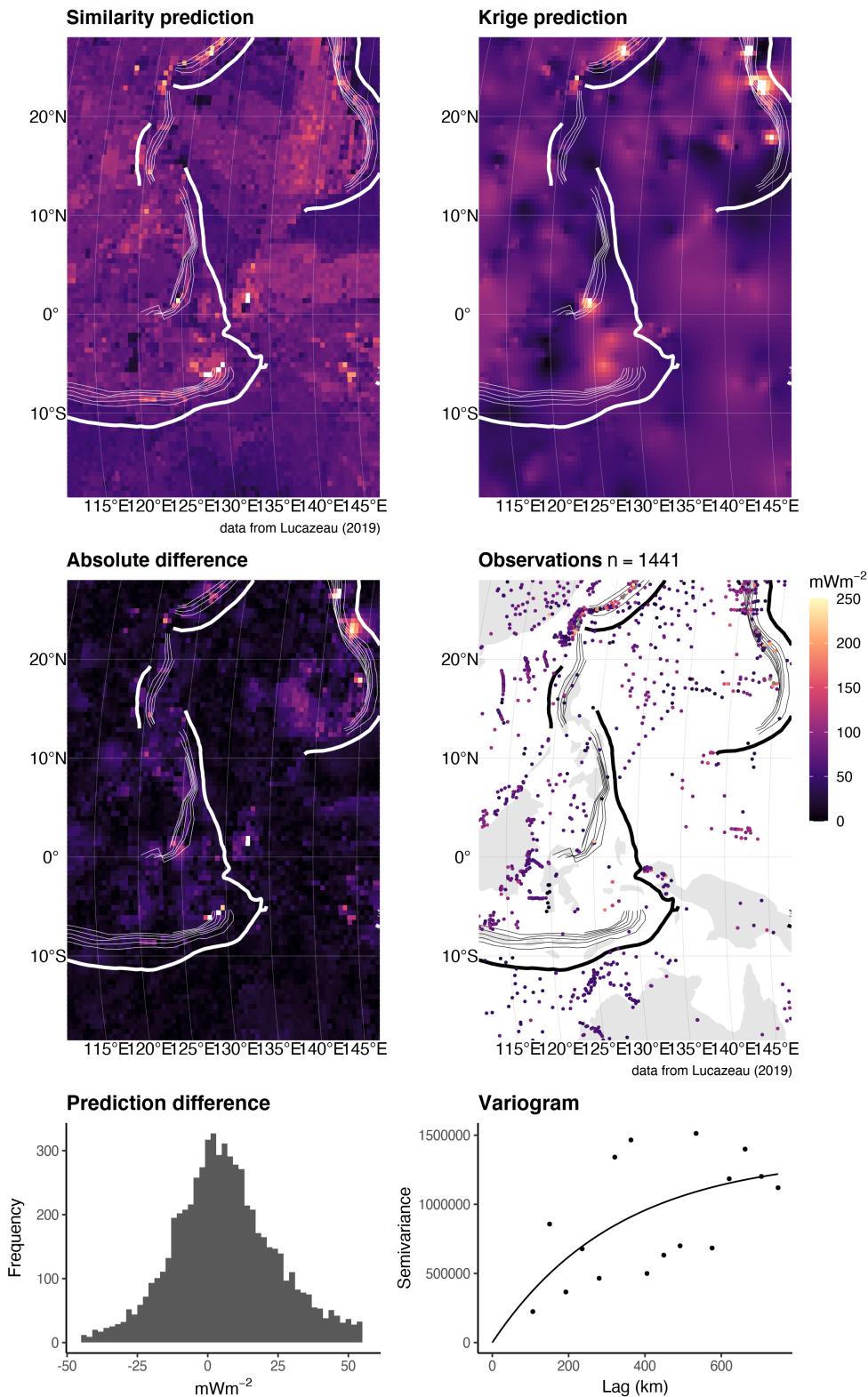


Figure 28: Similarity vs. Kriging predictions for S. Philippines. Kriging predictions are optimized by genetic algorithm.

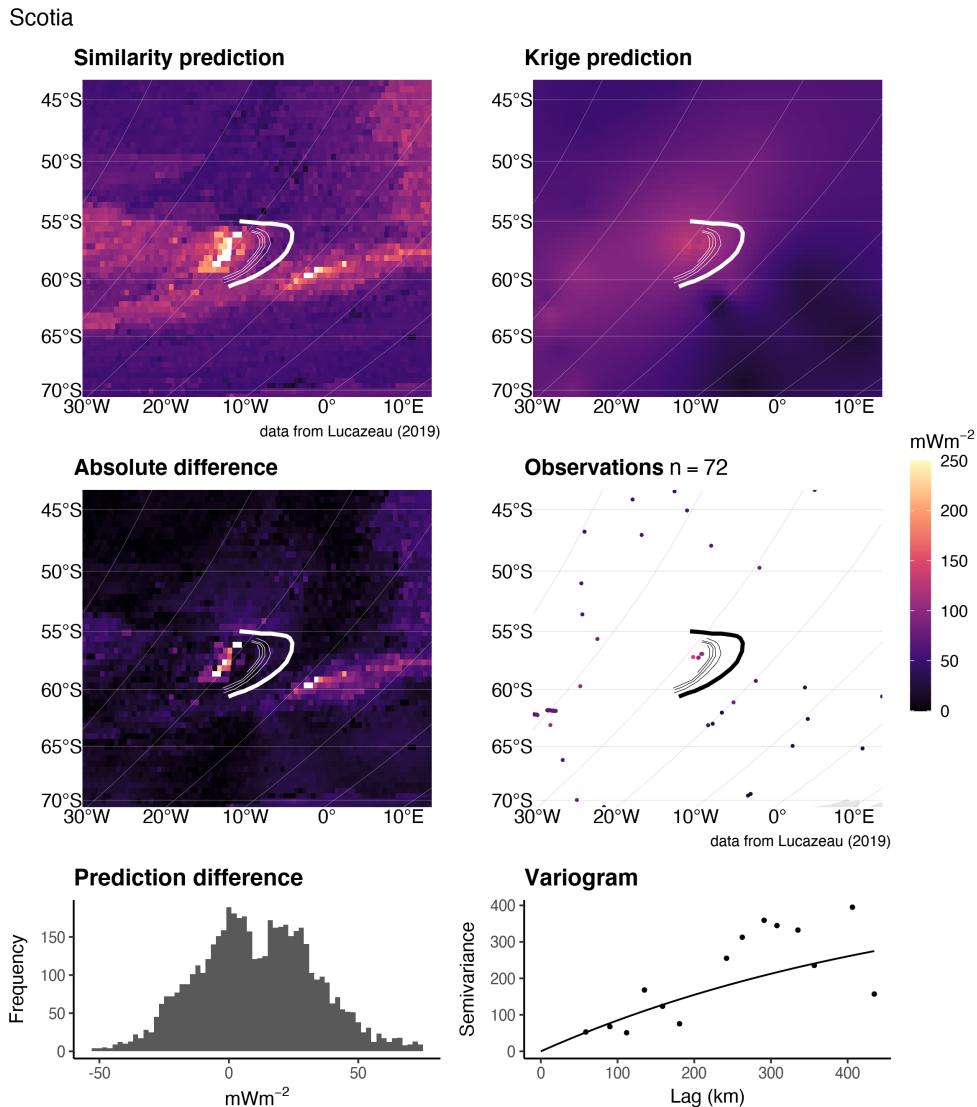


Figure 29: Similarity vs. Kriging predictions for Scotia. Kriging predictions are optimized by genetic algorithm.

Tonga New Zealand

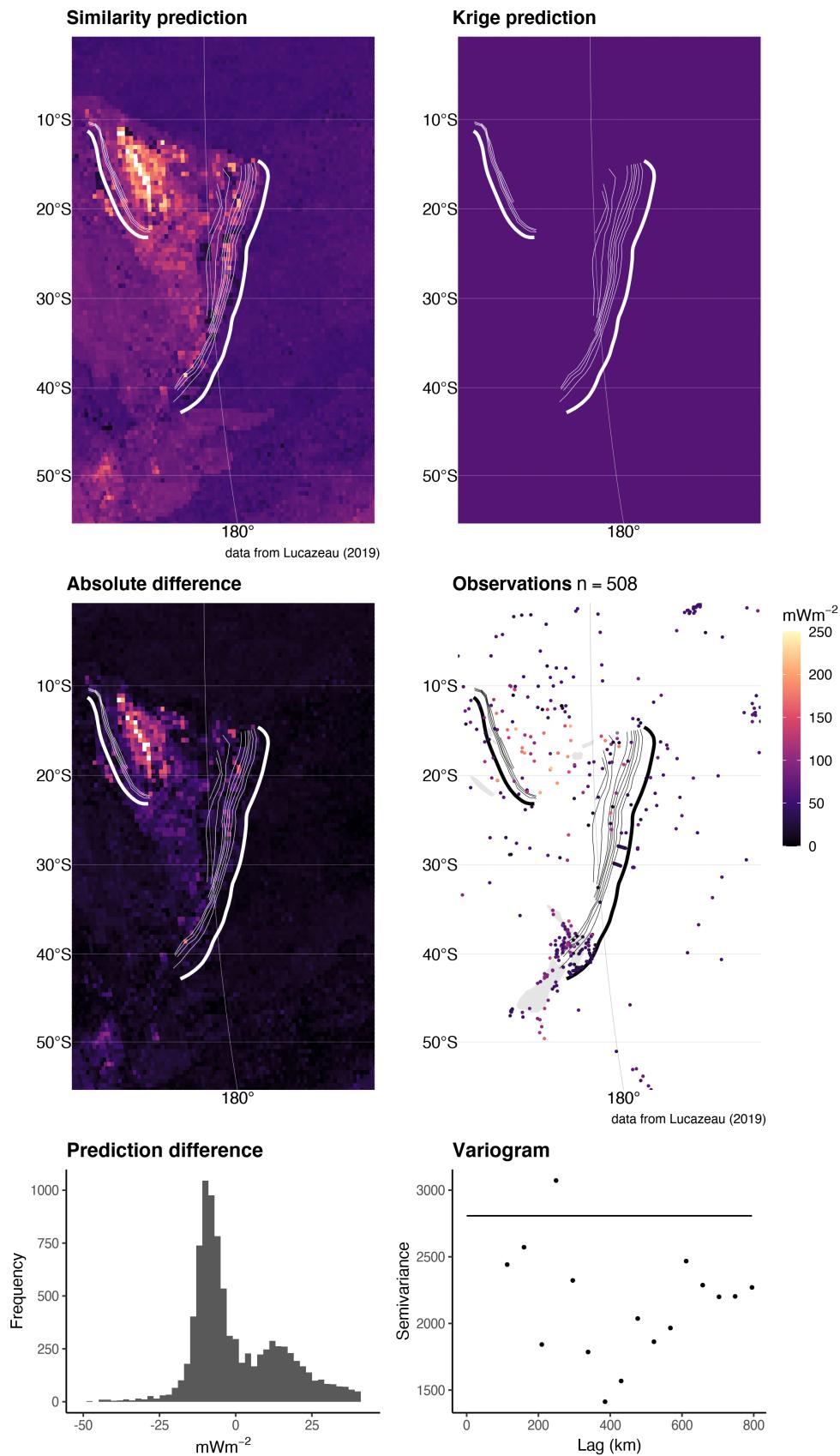


Figure 30: Similarity vs. Kriging predictions for Tonga New Zealand. Kriging predictions are optimized by genetic algorithm.

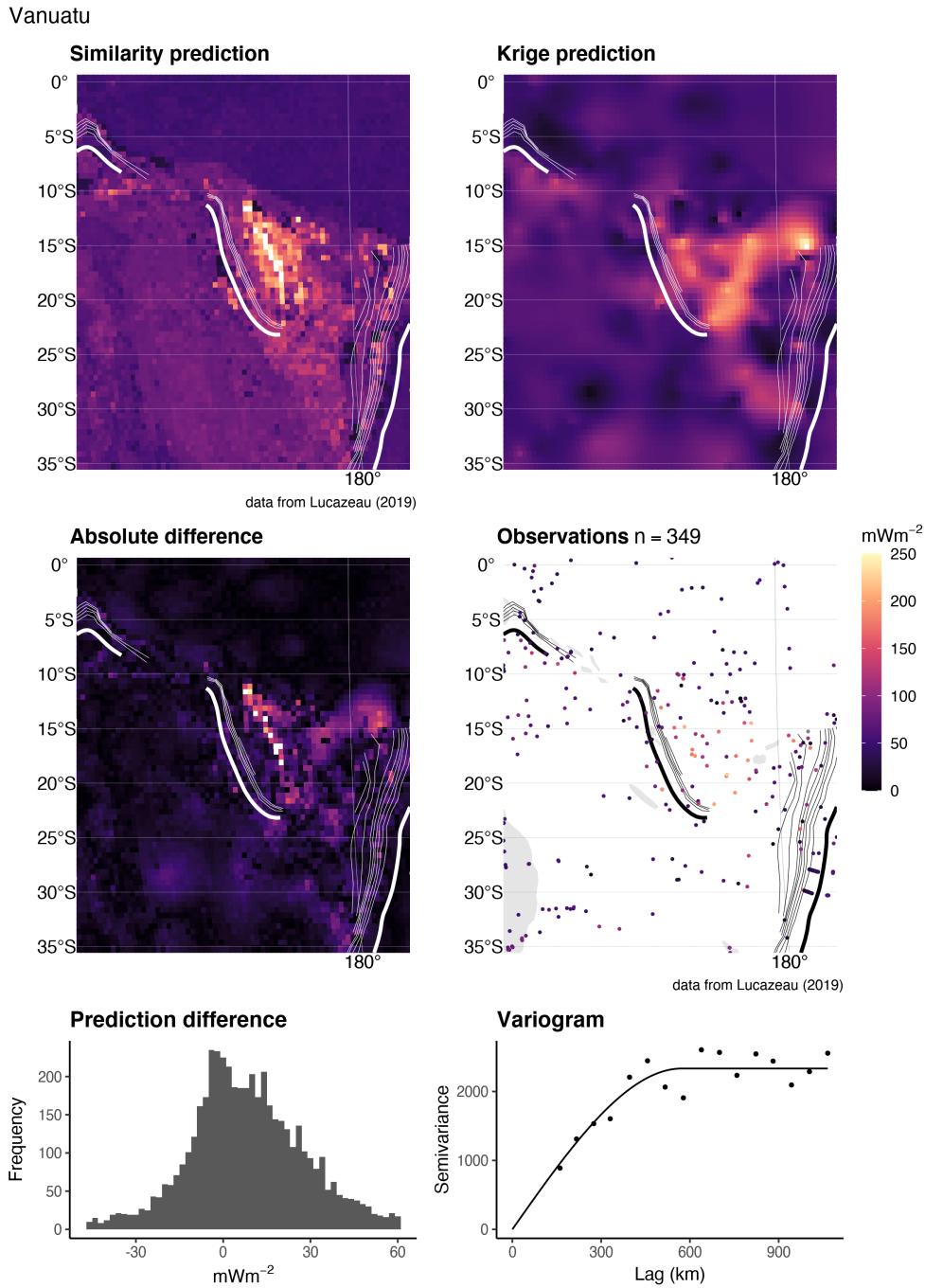


Figure 31: Similarity vs. Kriging predictions for Vanuatu. Kriging predictions are optimized by genetic algorithm.

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