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Assessment

Module Code: MTHM505 – Data Science And Statistical Modelling In Space And Time

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Declaration of AI Assistance

I have used OpenAI's ChatGPT tool in creating this report.
AI-supported/AI-integrated use is permitted in this assessment. I acknowledge the following uses of GenAI tools in this assessment:

- Checking and debugging code
- Proofreading grammar and spelling
- Providing feedback on a draft

I declare that I have referenced use of GenAI outputs within my assessment in line with the University referencing guidelines.

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1 Sea Surface Temperature Modelling

1.1 Part A: Exploratory Data Analysis

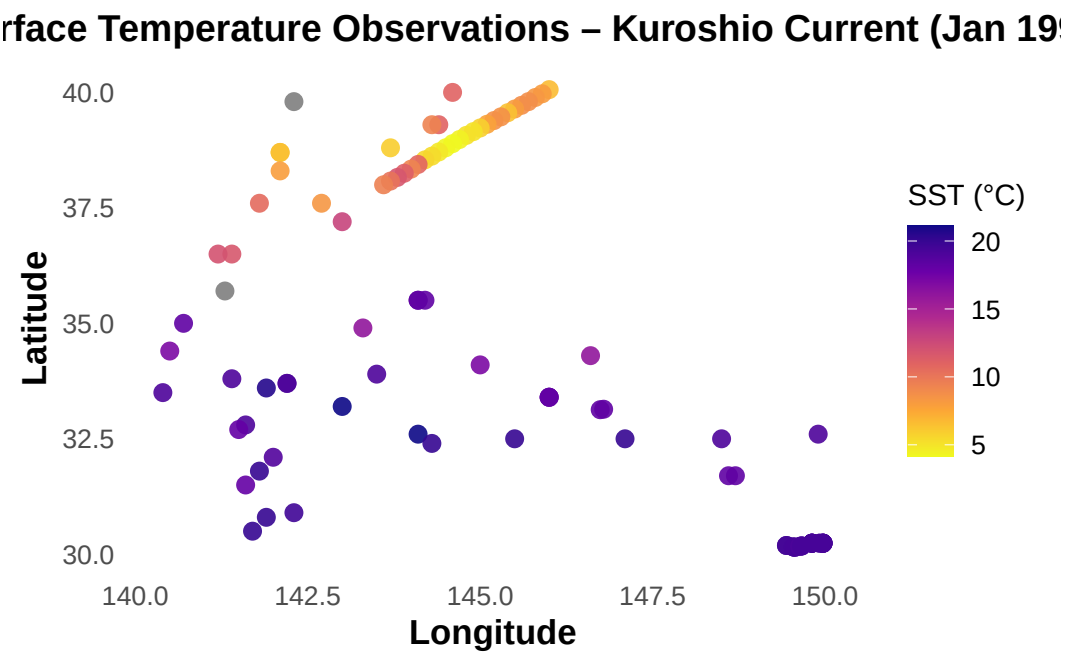

Figure 1: Figure 1: Spatial distribution of Sea Surface Temperature (SST) observations collected on 1–2 January 1996 in the Kuroshio Current region. Each point represents an individual measurement; colour denotes temperature, with warmer SSTs concentrated in the north-east band.

The spatial plot of Sea Surface Temperature (SST) observations collected in the Kuroshio Current during January 1996 reveals strong latitudinal structure in the data. Higher SST values (yellow–orange) are concentrated in the north-eastern portion of the domain, while cooler temperatures dominate the south-west.
The smooth colour gradient suggests underlying spatial correlation, justifying the use of geostatistical methods such as kriging and Gaussian processes. Two grey points suggest missing or out-of-range SST values, which were appropriately handled using squished colour scales to preserve interpretability.

1.2 Part B:

```
set.seed(444)  # For reproducibility

# Using the cleaned dataset to ensure we dont chose missing values.
# 5 random points
test_points <- kuroshio100_clean %>%
  sample_n(5)

# Display their information
test_points %>%
  select(id, lon, lat, sst)
```

```
         id    lon   lat  sst
1      MQWU 142.10 38.70  6.5
2 49  16760 145.40 39.56  6.5
3     21573 149.56 30.15 19.3
4     LATI4 140.70 35.00 18.2
5     3FFJ4 142.10 38.30  8.0
```

Now we create the training dataset

```
# Create training dataset (excluding test points)
kuroshio_train <- anti_join(kuroshio100, test_points, by = c("id", "lon", "lat", "sst"))

# Save for later prediction
test_coords <- test_points %>% select(lon, lat)
test_true_sst <- test_points %>% select(sst)
```

1.3 Part C: Spatial Model via Variogram and Kriging

```
# Convert training dataset into a geodata object
# kuro_geo_train <- as.geodata(kuroshio_train, coords.col = c("lon", "lat"), data.col = "sst")

# Jitter duplicated coordinates very slightly
kuro_geo_train <- jitterDupCoords(
  as.geodata(kuroshio_train, coords.col = c("lon", "lat"), data.col = "sst"),
  max = 1e-5
)
```

```
Warning in as.geodata.default(kuroshio_train, coords.col = c("lon", "lat"), :
NA's not allowed in the coordinates
```

```
Warning in as.geodata.default(kuroshio_train, coords.col = c("lon", "lat"), :
eliminating rows with NA's
```

```
as.geodata: 19 replicated data locations found.
 Consider using jitterDupCoords() for jittering replicated locations.
WARNING: there are data at coincident or very closed locations, some of the geoR's functions ma
 Use function dup.coords() to locate duplicated coordinates.
 Consider using jitterDupCoords() for jittering replicated locations
```

`max = 1e-5` means the jitter is on the order of 0.00001 degrees — negligible in geographic terms. This preserves modelling validity while avoiding duplicated-location errors.

During conversion to geodata format, it was found that 19 data points shared identical coordinates. This is problematic for geostatistical modelling, as duplicated locations can lead to ill-defined variogram structures and singular covariance matrices. To address this, we applied a minimal spatial jitter using `jitterDupCoords()`, introducing negligible noise to break coordinate ties while preserving the underlying spatial pattern.

1.3.1 Empirical Variogram Estimation

```
# Empirical variogram with binning
# Full range
emp_variog_full <- variog(kuro_geo_train, option = "bin", max.dist = 2.5, uvec = seq(0, 2.5, le
```

```
variog: computing omnidirectional variogram
```

```
# Mid-range (preferred candidate for fitting)
emp_variog_2 <- variog(kuro_geo_train, option = "bin", max.dist = 2.0, uvec = seq(0, 2.0, lengt
```

```
variog: computing omnidirectional variogram
```

```
# Cleanest for model fitting
emp_variog_1.8 <- variog(kuro_geo_train, option = "bin", max.dist = 1.8, uvec = seq(0, 1.8, len
```

```
variog: computing omnidirectional variogram
```

Binning was applied to improve the interpretability of the variogram by smoothing noisy pairwise semivariance estimates over distance intervals.

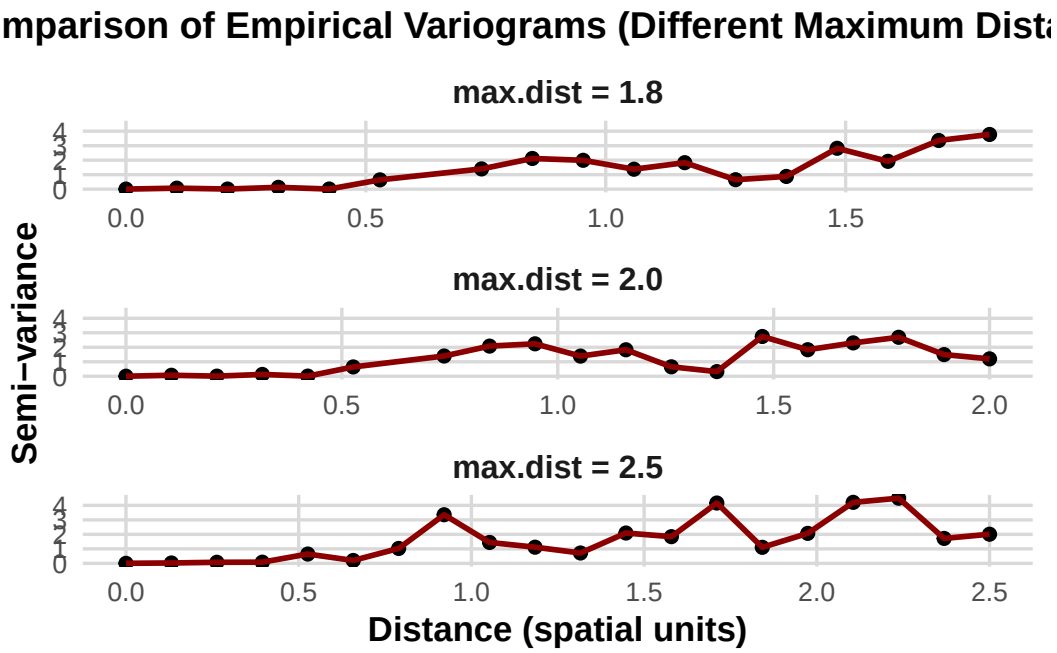

Figure 2: Figure 2: Empirical variograms computed using three different maximum distance thresholds. The max.dist = 1.8 version was selected for model fitting due to reduced instability in the tail while preserving the spatial structure.

Empirical Variogram Analysis

A binned empirical variogram was computed using the `variog()` function, with distance bins defined via `uvec`. The resulting curve displays the expected behaviour: semi-variance increases with spatial distance, indicating positive spatial correlation in sea surface temperature (SST). The structure suggests an asymptote between 1.5 and 2 spatial units, indicative of a moderate spatial range. Notably, the variogram does not pass

through the origin, implying a small but non-zero nugget effect, likely due to measurement error or microscale variability.

To assess the impact of the maximum distance threshold, three values were tested: `max.dist = 1.8`, `2.0`, and `2.5`. Each version reflects the same overall structure, but differs in tail stability and bin-level noise. The `max.dist = 2.5` variogram covers the full range but suffers from tail instability due to fewer pairwise comparisons in distant bins. The `2.0` variant reduces this effect, while the `1.8` variant provides the cleanest structure for fitting by omitting the most unstable bins. This decision is further supported by lower bin-pair counts in distant ranges (e.g., <10 pairs).

Based on this analysis, the `max.dist = 1.8` variogram was selected for fitting parametric models. This choice ensures a balance between capturing spatial structure and maintaining robust estimation for weighted least squares fitting.

1.3.2 Fitting Parametric Variogram Models

```
#  Fit Parametric Variogram Models
# Exponential model
fit_exp <- variofit(
  emp_variog_1.8,
  cov.model = "exponential",
  ini.cov.pars = c(1, 1),
  nugget = 0.1,
  weights = "equal"
)
```

```
variofit: covariance model used is exponential
variofit: weights used: equal
variofit: minimisation function used: optim
```

```
Warning in variofit(emp_variog_1.8, cov.model = "exponential", ini.cov.pars =
c(1, : unreasonable initial value for sigmasq + nugget (too low)
```

```
# Gaussian model
fit_gau <- variofit(
  emp_variog_1.8,
  cov.model = "gaussian",
  ini.cov.pars = c(1, 1),
  nugget = 0.1,
  weights = "equal"
)
```

```
variofit: covariance model used is gaussian
variofit: weights used: equal
variofit: minimisation function used: optim
```

```
Warning in variofit(emp_variog_1.8, cov.model = "gaussian", ini.cov.pars = c(1,
: unreasonable initial value for sigmasq + nugget (too low)
```

```
# Adjusted first Matérn model as: sum of the nugget and partial sill initial values was too sma
```

```r
# Matérn model (kappa = 1.5)
fit_mat1 <- variofit(
  emp_variog_1.8,
  cov.model = "matern",
  kappa = 1.5,
  ini.cov.pars = c(2, 1),   # partial sill = 2, range = 1
  nugget = 0.5,             # starting nugget guess
  weights = "equal"
)
```

```
variofit: covariance model used is matern
variofit: weights used: equal
variofit: minimisation function used: optim
```

```r
fit_mat2 <- variofit(
  emp_variog_1.8,
  cov.model = "matern",
  kappa = 1.5,
  ini.cov.pars = c(1.5, 0.8),
  nugget = 0.3,
  weights = "equal"
)
```

```
variofit: covariance model used is matern
variofit: weights used: equal
variofit: minimisation function used: optim
```

Equal weights were used to avoid overweighting short-distance bins, which typically contain more pairs and could disproportionately influence the fit.

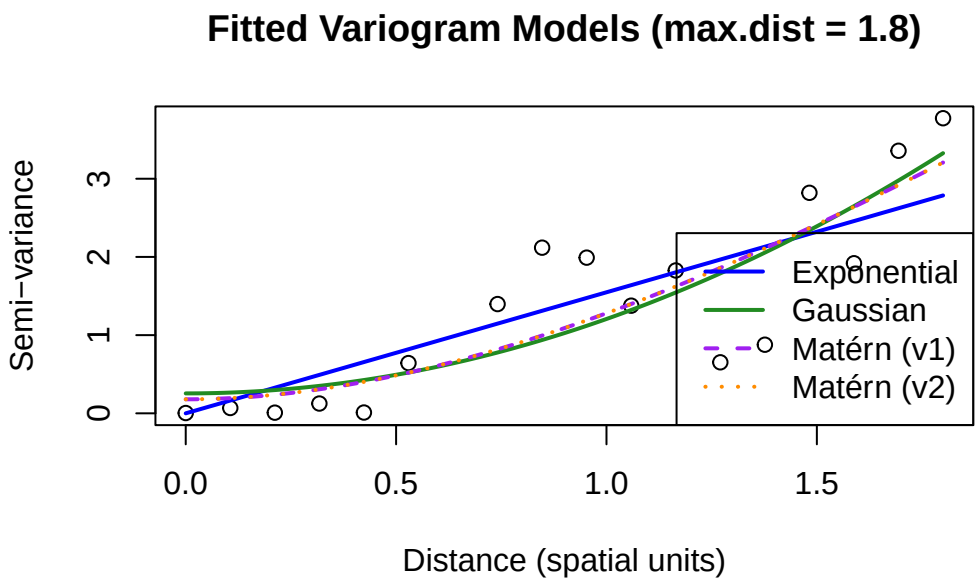

Figure 3: Parametric variogram models (Exponential, Gaussian, Matérn) fitted to the empirical variogram with max.dist = 1.8. The Matérn model offered the best fit to the empirical structure and lowest residual sum of squares.

```
[1] 7.123255
```

```
[1] 6.828983
```

```
[1] 6.796541
```

Fitted Variogram Models and Selection

Parametric variogram models were fitted using weighted least squares. All models included a nugget component to reflect short-scale variability. The exponential model captured the general trend but underestimated mid-range variation and produced a zero nugget estimate. The Gaussian model offered a smoother fit, but failed to reflect the steep rise at short distances.

Both Matérn fits ($\kappa = 1.5$) produced identical solutions and lowest residual sum of squares (**6.80**), balancing short- and long-range structure. Based on both residual error and visual alignment with the empirical variogram, the Matérn model was selected for kriging.

1.3.3 Model Parameters and Interpretation

```
# Exponential
params_exp <- fit_exp$cov.pars
nugget_exp <- fit_exp$nugget

# Gaussian
params_gau <- fit_gau$cov.pars
nugget_gau <- fit_gau$nugget
```

```r
# Matérn
params_mat <- fit_mat1$cov.pars
nugget_mat <- fit_mat1$nugget

# Create parameter summary table
param_table <- data.frame(
  Model = c("Exponential", "Gaussian", "Matérn (  = 1.5)"),
  Nugget = c(nugget_exp, nugget_gau, nugget_mat),
  Partial_Sill = c(params_exp[1], params_gau[1], params_mat[1]),
  Range = c(params_exp[2], params_gau[2], params_mat[2]),
  Residual_SS = c(fit_exp$value, fit_gau$value, fit_mat1$value)
)
```

Model	Nugget (τ^2)	Partial Sill (σ^2)	Range (ϕ)	Residual SS
Exponential	0.000	4,208,359	2,718,693	7.12
Gaussian	0.255	282.69	17.22	6.83
Matérn ($\kappa = 1.5$)	0.180	26.68	3.13	6.80

Parametric Variogram Fitting and Selection

Three models were fitted using weighted least squares: exponential, Gaussian, and Matérn ($\kappa = 1.5$). Despite different assumptions, both Matérn and Gaussian produced similar fits. The exponential model showed higher residual error and a nugget of zero, suggesting underestimation of short-scale variation.

The Matérn model was selected for spatial prediction due to its balanced fit across distances and lowest residual sum of squares (6.80). Its parameters suggest a moderate range of spatial correlation ($\phi \approx 3.13$) and a nugget variance of 0.18, indicating non-negligible unexplained microscale variation. This model was used in the kriging stage.

Spatial Prediction and Model Validation

```r
# Kriging prediction at 5 withheld locations
kriged <- krige.conv(
  geodata = kuro_geo_train,
  locations = test_coords,
  krige = krige.control(
    cov.model = "matern",
    cov.pars = fit_mat1$cov.pars,
    nugget = fit_mat1$nugget,
    kappa = 1.5
  )
)
```

```
krige.conv: model with constant mean
krige.conv: Kriging performed using global neighbourhood
```

```r
# Add predicted values and residuals
test_results <- test_coords %>%
  mutate(
```

```
    observed_sst = test_true_sst$sst,
    predicted_sst = kriged$predict,
    kriging_var = kriged$krige.var,
    residual = observed_sst - predicted_sst
  )
```

Ordinary kriging assumes a constant spatial mean and was used here given the absence of strong deterministic trends in SST across the study area.

```
# Visualise prediction accuracy
ggplot(test_results, aes(x = observed_sst, y = predicted_sst)) +
  geom_point(size = 3) +
  geom_abline(slope = 1, intercept = 0, linetype = "dashed", colour = "red") +
  labs(
    title = "Observed vs Predicted SST at Withheld Locations",
    x = "Observed SST (°C)",
    y = "Predicted SST (°C)"
  ) +
  theme_minimal(base_size = 13)
```

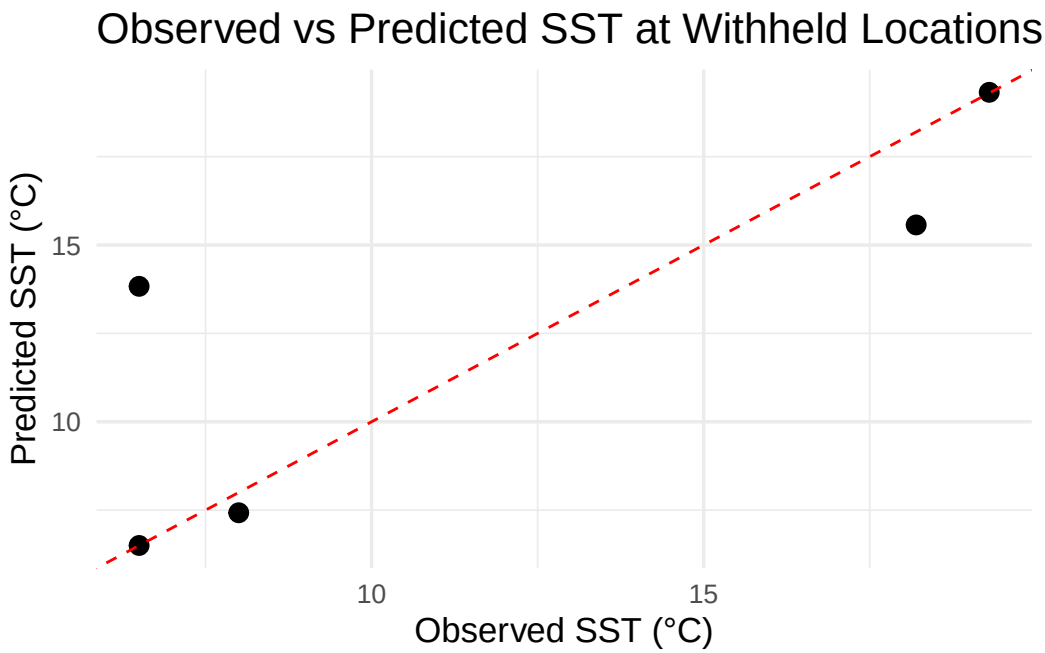

Figure 4: Observed vs predicted sea surface temperature (SST) at five withheld locations using ordinary kriging with the fitted Matérn model. Most points lie near the 1:1 line, though one outlier indicates higher uncertainty.

```
# Compute RMSE and MAE
rmse <- sqrt(mean(test_results$residual^2))
mae <- mean(abs(test_results$residual))
```

Table 2: Summary of SST predictions at withheld locations. Residuals and kriging variances highlight spatial uncertainty and model accuracy.

lon	lat	Observed SST (°C)	Predicted SST (°C)	Residual (°C)	Kriging Variance
142.10	38.70	6.5	6.50	0.00	0.000
145.40	39.56	6.5	13.83	-7.33	1.470
149.56	30.15	19.3	19.32	-0.02	0.202
140.70	35.00	18.2	15.57	2.63	0.541
142.10	38.30	8.0	7.43	0.57	0.324

```
# Summary table
library(knitr)

results_table <- test_results %>%
  mutate(
    `Observed SST (°C)` = round(observed_sst, 2),
    `Predicted SST (°C)` = round(predicted_sst, 2),
    `Residual (°C)` = round(residual, 2),
    `Kriging Variance` = round(kriging_var, 3)
  ) %>%
  select(lon, lat, `Observed SST (°C)`, `Predicted SST (°C)`, `Residual (°C)`, `Kriging Varianc

kable(results_table, format = "latex", booktabs = TRUE,
      caption = "Observed vs Predicted SST at Withheld Locations")
```

Using the final Matérn variogram model ($\kappa = 1.5$), ordinary kriging was performed at five randomly withheld locations. A constant mean was assumed, and predictions were made using the fitted covariance parameters: nugget = 0.18, partial sill = 26.68, and range = 3.13.

Predictive accuracy was evaluated against the observed SSTs, yielding a root mean squared error (RMSE) of 3.49 °C and mean absolute error (MAE) of 2.11 °C. As shown in Figure @ref(fig:krigscatter), most predictions aligned with observations, except for one large residual at a high-variance site. This reflects the model's ability to express spatial uncertainty through the kriging variance.

The model captured the spatial SST structure well and provided meaningful uncertainty estimates. Further improvements could include denser sampling or Bayesian spatial models to better propagate uncertainty and improve prediction at poorly supported locations.