# something

FEM11149 - Introduction to Data Science

Maya Archer 623099 (25%), Nicolas Gonzalez Gort 780037 (25%)
Rishi Ashok Kumar 560527 (25%), Saumya Bothra 595402 (25%)

## Introduction

Short horizon temperature forecasts inform planning in energy, transport, public health, and city services, where load balancing, maintenance, and emergency response depend on credible next-day expectations. Utilities, grid operators, and municipalities translate such forecasts into operational budgets, staffing, and risk management strategies. Scientifically, multiple drivers shape daily maximum temperature- surface energy balance (radiative fluxes, cloud cover, albedo), boundary-layer dynamics (humidity, wind speed, mixing), seasonal cycles, and urban heat-island effects- the joint behavior of which exhibits collinearity and regime dependence. Hence, the need to identify useful predictors for next-day maxima and compress them without sacrificing accuracy, leading to the central research question of this study: *To what extent does PCA-based feature extraction improve next-day maximum-temperature prediction when evaluated out-of-sample and across different target regimes?* The results of this analysis aim to clarify which compressed structures carry predictive signal, informs adoptable model choices for short-horizon operations, and indicates where forecasts degrade across regimes.

## Data

Daily weather observations from the Copernicus Regional Reanalysis for Europe (CERRA) are used for Rome, yielding 4,020 days (~12 years). The dependent variable is next day daily maximum temperature in °C. The independent variables include all numeric meteorological variables observed on day $t$; including the circular angle `dominant_wind_direction` (0–360°) as is and the same-day `max_temperature_c` as a lagged regressor for forecasting day *t+1*. Initial summary statistics show that temperature levels center around mean 20.90 °C, with average perceived measures averaged at 15.43 °C and average perceived max temperatures at 20.52 °C. Wind intensity is moderate on average at 15.26 km/h. Average radiative and evapotranspiration processes show clear seasonality (15.69 MJ/m², 3.03 mm), with photoperiod measures confirming winter–summer contrast- where the average daylight duration is 12.21 h. Hydrometeorological activity averages are low but episodic. Average precipitation lands at 2.44 mm, where the average rainfall lands at 2.43mm, consistent with many dry days punctuated by occasional events.

## Methodology

Some common notation in the following methodolgy are as follows. $y_t$ denotes the daily maximum temperature (°C) on day $t$ and $X_t \in \mathbb{R}^p$ is the vector of meteorological predictors observed on day $t$. The one day ahead forecasting is done through supervised regression using aligned pairs $\{(X_t, y_{t+1})\}_{t=1}^{T-1}$ in which the response variable is $y_{t+1}$ = `max_temperature_c` on the next day, and the predictors are the full numeric feature set on day $t$ including the same-day `max_temperature_c` as a lagged regressor and the circular angle `dominant_wind_direction` (0–360°) included untransformed.

The baseline linear model which also serves as the benchmark in this analysis is an Ordinary Least Squares (OLS) model

$$y_{t+1} = \beta_0 + \sum_{j=1}^{p} \beta_j X_{t,j} + \varepsilon_{t+1},$$

While OLS provides interpretable results, it is sensitive to multi-collinearity among meteorological variables (e.g., temperature levels and perceived temperatures, radiation and evapotranspiration). The OLS model is trained on the training set and evaluated on the test set, the demarcation of which is later specified. $R^2$ and RMSE is are used for comparison.

A Principal Component Analysis (PCA) is applied on the training predictors, after centering means and scaling variances. PCA focuses primarily on de-correlation and dimensional reduction under strong multi-collinearity, as mentioned above. While it is not tailored to extremes, it provides an independent basis for stable regression and clear diagnostics. With training matrix $X_{\text{train}} \in \mathbb{R}^{n \times p}$, PCA computes the decomposition $X_{\text{train}} = UDV^\top$. Columns of $V$ are the loadings and the principal component scores are $Z = X_{\text{train}}V$. The variance explained by the $k$ leading components is $\text{VAF}_k = \sum_{j=1}^{k} d_j^2 / \sum_{j=1}^{p} d_j^2$. In this study, the diagnostic checks include the scree plot, a cumulative Variance Acounted For (VAF) curve, biplots for (PC1, PC2) & (PC2, PC3), and loading tables to interpret variable groupings.

In order to choose the number of components, three main methods are applied on the training set- a cumulative VAF threshold at $\geq 85\%$), The Kaiser's rule where eigenvalues $> 1$, and a parallel (permutation) analysis comparing real eigenvalues to those from column wise permuted data. The main model also conducts sensitivity checks at $k-1$ and $k+1$, to assess robustness of predictive results to the retention level.

Sampling variability in $\text{VAF}_k$ is quantified by nonparametric bootstrapping, where rows of $X_{\text{train}}$ are resampled $B = 1000$ times. PCA is then recomputed on each bootstrap sample, and $\text{VAF}_k$ is aggregated to form a sampling distribution. A 95% percentile confidence interval is reported. This procedure is performed on training data to avoid test leakage.

The principal component analysis regresses the response on the first $k$ PC scores:

$$y_{t+1} = \alpha_0 + \sum_{j=1}^{k} \gamma_j Z_{t,j} + \eta_{t+1}, \qquad Z_t = X_t V_{(:,1:k)}.$$

The rotation $V$ and training centering/scaling parameters are frozen and applied to $X_{\text{test}}$ to obtain test scores before prediction.

For this analysis, a contiguous 80/20 split is performed. The first 80% of aligned pairs form the training set and the final 20% form the test set used only once for final evaluation. All data-dependent transformations such as scaling and PCA rotations are estimated on the training set and then applied to the test set.

Prior to modeling, linear associations between each predictor in $X_t$ and the target $y_{t+1}$ are examined using Pearson correlations and scatter plots with OLS trend lines. These diagnostics motivate the use of PCA and provide context for interpreting early component loading.

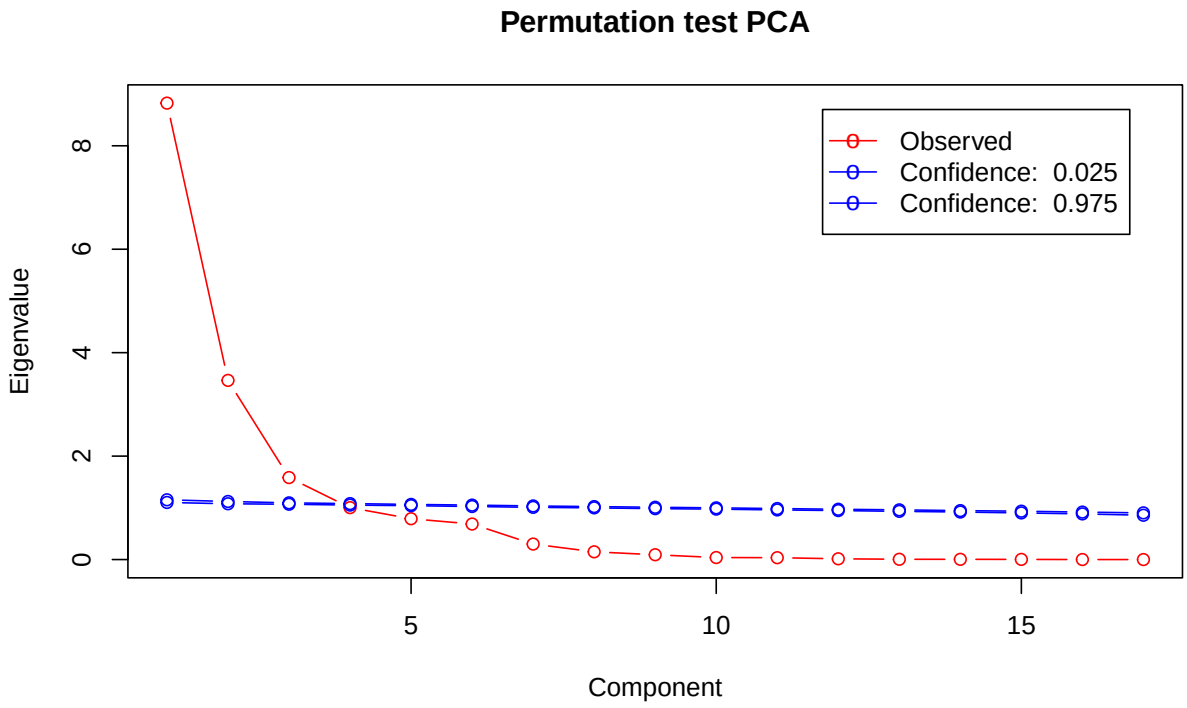
The model's predictive accuracy is assessed on the test set using Root Mean Squared Error (RMSE) as the primary metric and the $R^2$ is provided for context. To examine regime dependence, test observations are partitioned into deciles of the observed $y_{t+1}$, and the RMSE by each decile is reported for the OLS and PCA model specifications, indicating whether errors concentrate in colder or hotter ranges. Random seeds are set for reproducibility of re-sampling and permutation steps.

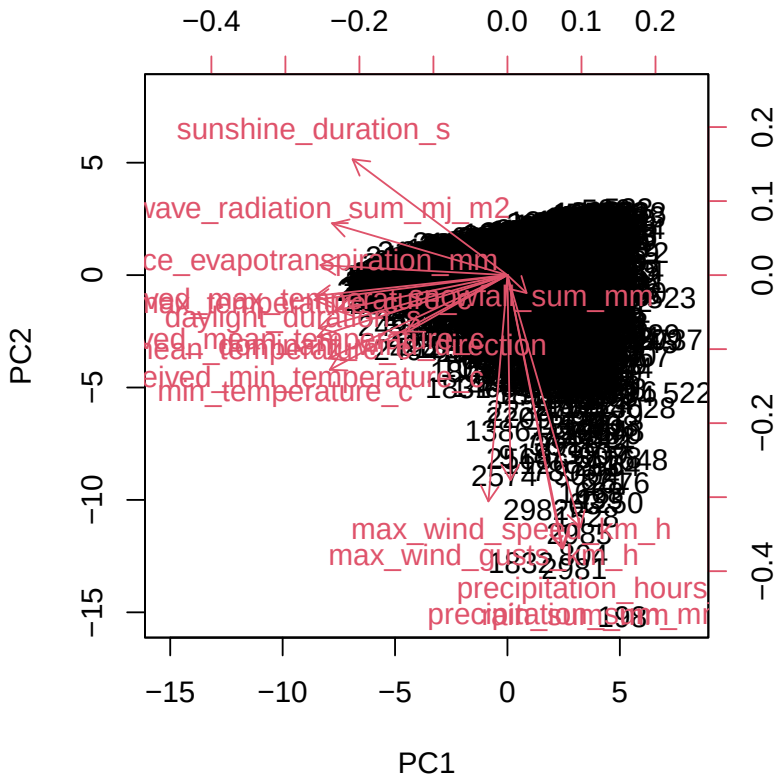
# Results

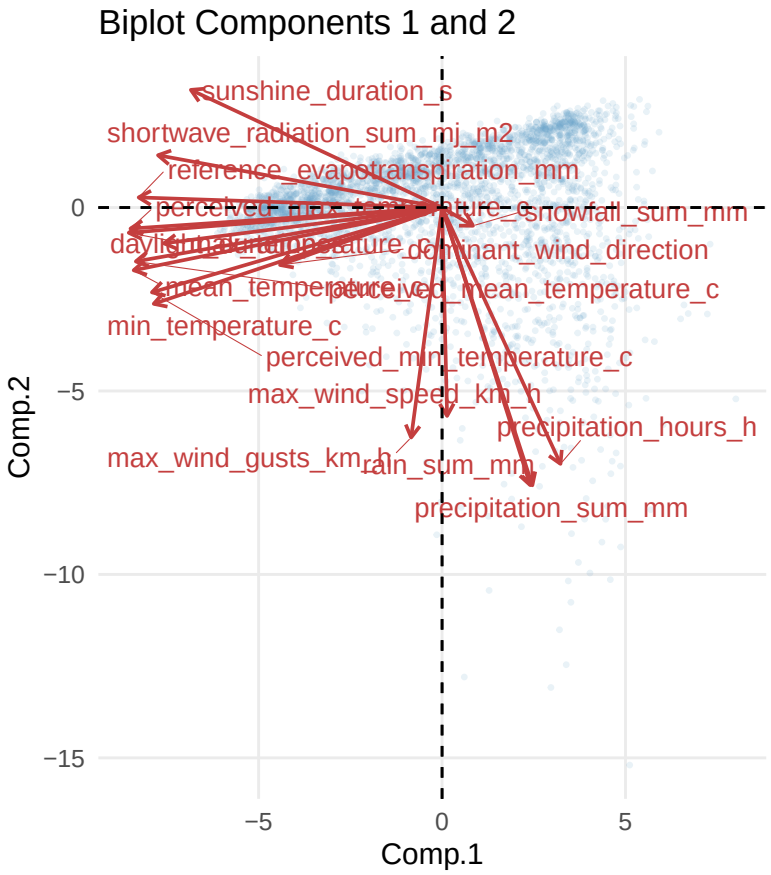
Table 1 (Appendix A) shows that next-day maximum temperature is strongly correlated to same-day thermal conditions: higher current max/mean/min (and their perceived counterparts) go hand-in-hand with hotter tomorrows. Seasonal and surface-energy indicators (sunshine, daylight, shortwave radiation, and reference

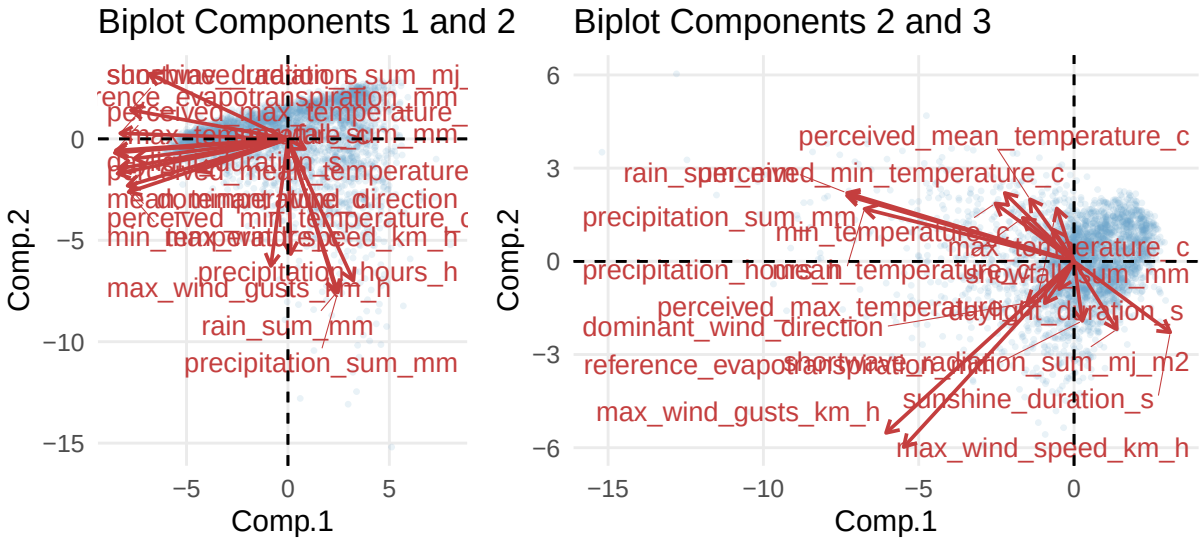
evapotranspiration) move in the same direction, pointing to a "clear, dry, sunny" pattern that precedes warmer days. In contrast, precipitation works in the opposite way, meaning that more hours or larger sums of rain today are followed by lower next-day temperatures. Wind variables don't show any strong effects. The scatterplots in Figure 1 confirm these results showing positive, near-linear trends for temperature and radiation, and downward slopes for precipitation.

To avoid look-ahead bias, we estimated Principal Components Analysis only on the training dataset and froze its rotation and scaling. Figure X shows a sharp elbow with eigenvalues for PC1-PC4 of 8.82, 3.46, 1.59, 1.00, respectively (Table 2). By the third component we already explain about 82% of the variance, with only a small gain if a fourth is added (up to 88%), which can be seen in Table 3. The two selection rules point in slightly different directions: Kaiser would keep 4 components, while parallel analysis (permutation cut-offs) is more conservative with k = 3. Balancing parsimony and coverage, we adopt 3 components as the baseline for prediction and treat the fourth as an optional robustness check.




−0.4
−0.2
0.0
0.1
0.2
sunshine_duration_s
wave_radiation_sum_mj_m2
ce_evapotranspiration_mm
daylight_duration
min_temperature_c
max_wind_speed_10m_h
precipitation_hours
PC2
PC1
5
0
−5
−10
−15
0.2
0.1
0.0
−0.2
−0.4


Biplot Components 1 and 2
sunshine_duration_s
shortwave_radiation_sum_mj_m2
reference_evapotranspiration_mm
snowfall_sum_mm
dominant_wind_direction
mean_temperature_c
perceived_mean_temperature_c
min_temperature_c
perceived_min_temperature_c
max_wind_speed_km_h
precipitation_hours_h
max_wind_gusts_km_h
rain_sum_mm
precipitation_sum_mm
0
−5
−10
−15
−5
0
5
Comp.2
Comp.1


Biplot Components 1 and 2
Comp.2
Comp.1
0
−5
−10
−15
5
precipitation_hours_h
max_wind_gusts_km_h
rain_sum_mm
precipitation_sum_mm
Biplot Components 2 and 3
Comp.2
Comp.1
6
3
0
−3
−6
−15
−10
−5
0
perceived_mean_temperature_c
precipitation_sum_mm
dominant_wind_direction
max_wind_gusts_km_h
sunshine_duration_s
max_wind_speed_km_h

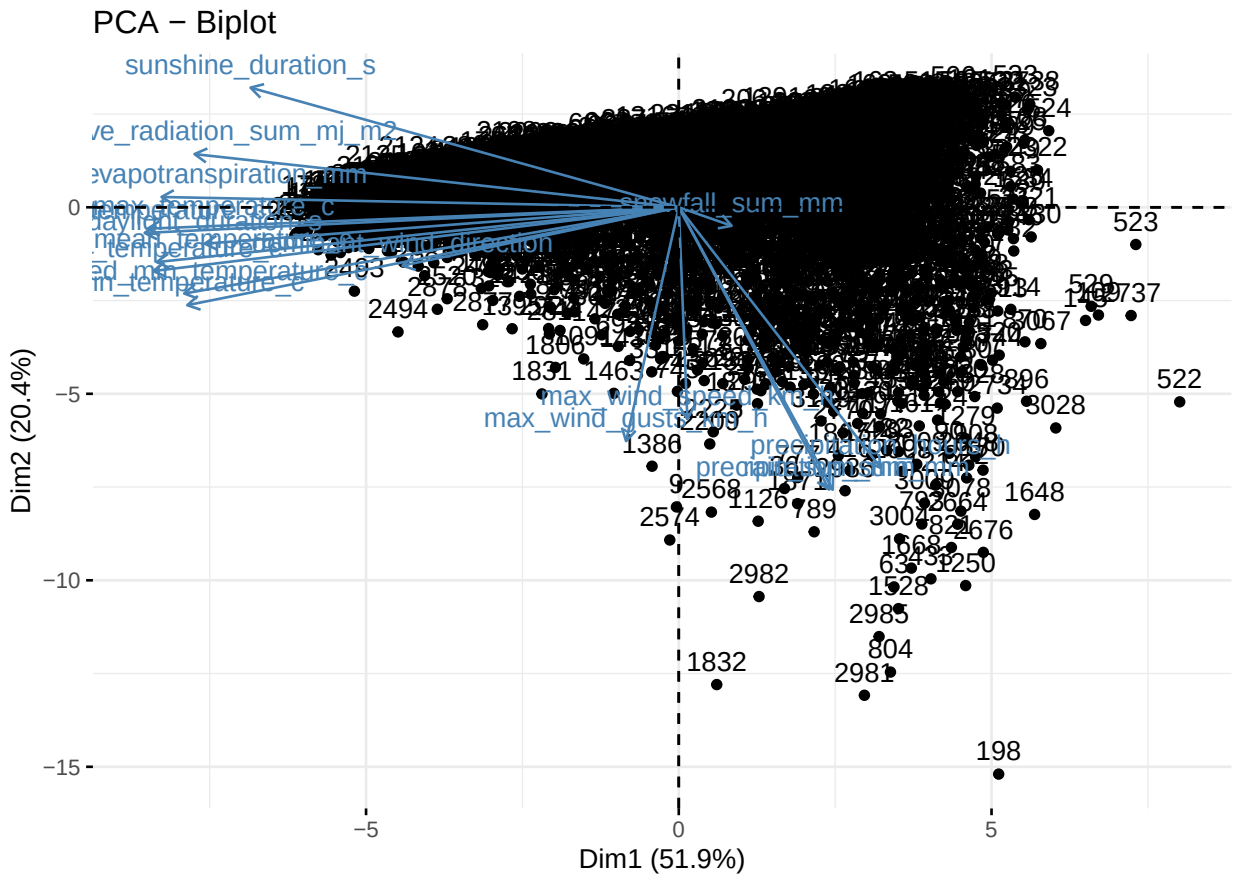



Table 5 shows the PCA reduction of weather variables into three interpretable dimensions. The first component acts like a "seasonality/heat" axis: it loads in the same direction on actual and perceived temperatures, sunshine, shortwave radiation, daylight, and evapotranspiration, with the opposite sign on precipitation, effectively contrasting warm, sunny, dry days with cool, wet, overcast ones. The second component reflects precipitation intensity with gustiness, distinguishing short, heavy rainfall episodes that coincide with stronger gusts from longer, lighter precipitation under calmer winds. The third captures wind strength versus warmth, separating windy–cool from calm–warm conditions and being driven primarily by wind speed and gusts with lighter temperature contributions. Communalities indicate that the best-represented variables in the k = 3 subspace are actual and perceived temperatures (max_temperature_c, mean_temperature_c, perceived_max_temperature_c, perceived_mean_temperature_c), together with radiative and photoperiod indicators (shortwave_radiation_sum_mj_m2, daylight_duration_s, sunshine_duration_s) and reference_evapotranspiration_mm. Snowfall, precipitation hours, and dominant_wind_direction are least represented. We retain three components because the scree flattens after the third, the parallel-analysis cutoff aligns with a conservative choice of three, and cross-validated PCR error improves up to k = 3 with small gains after. In addition, the first three components together account for about 82% of the variance (bootstrap 95% CI = 81.1–82.1%), so the dimensionality reduction is reliable and not driven by a particular sample split.

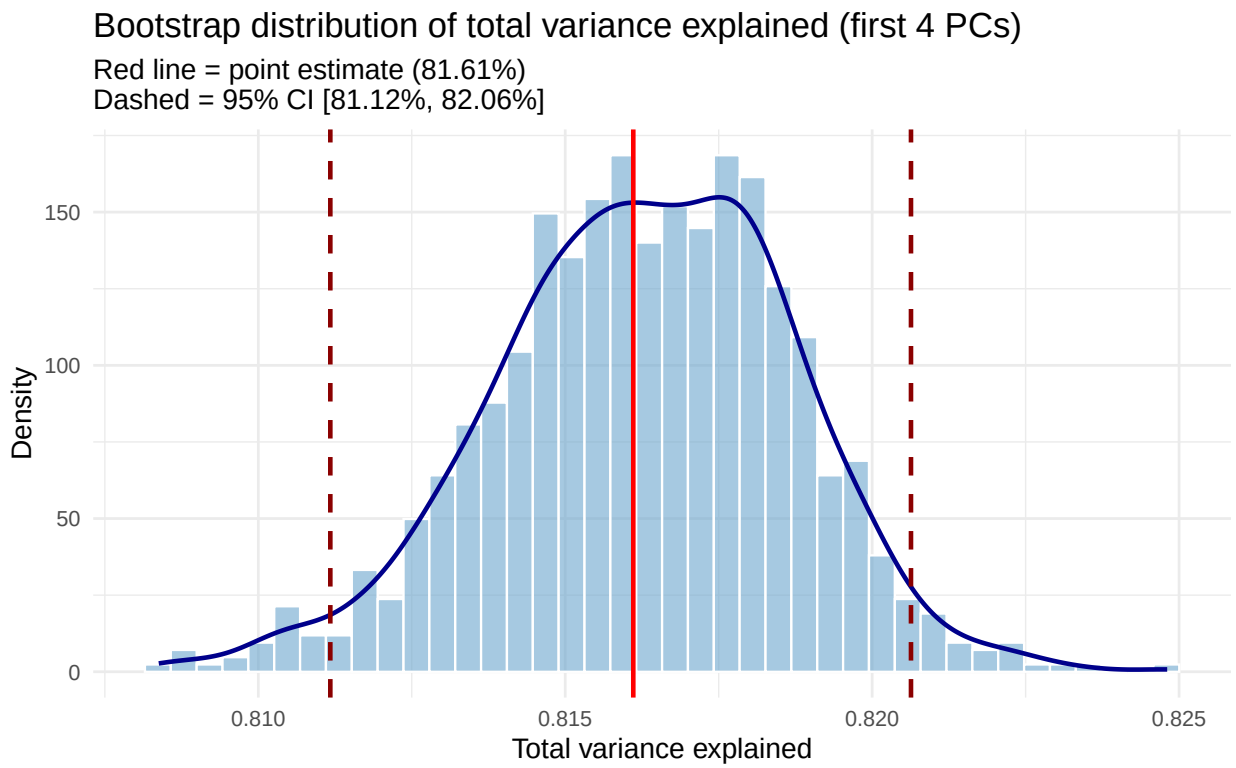
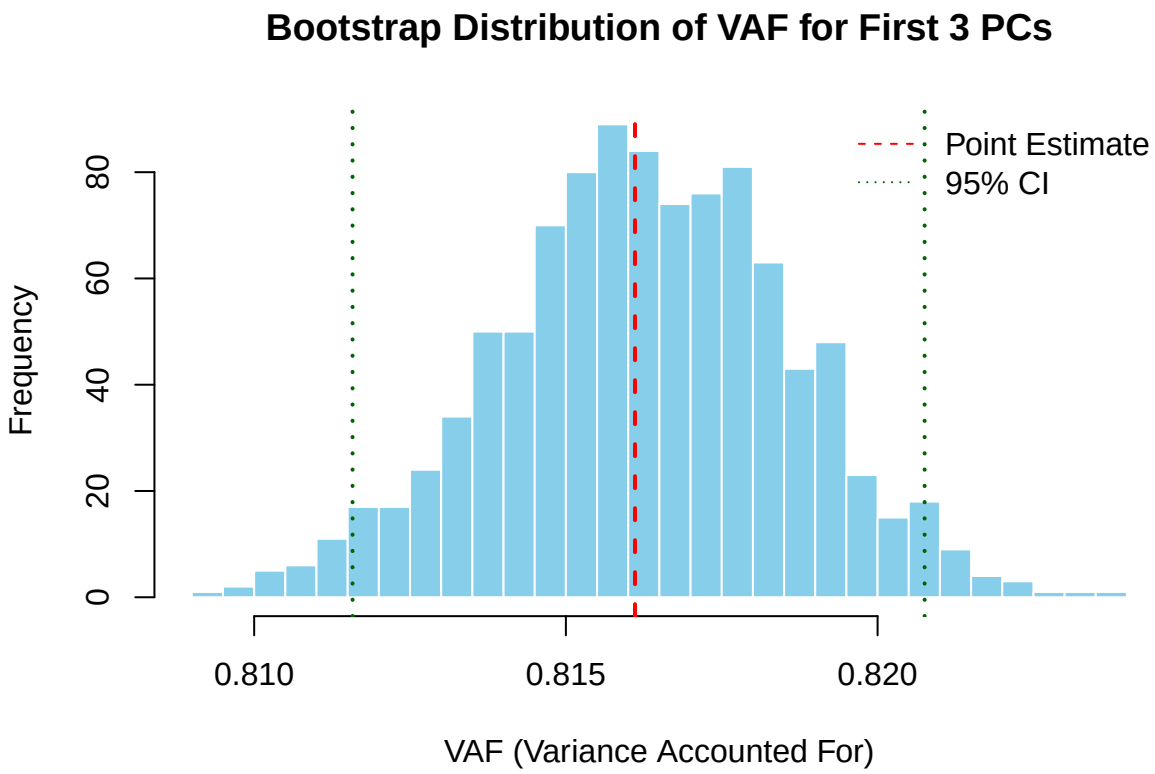
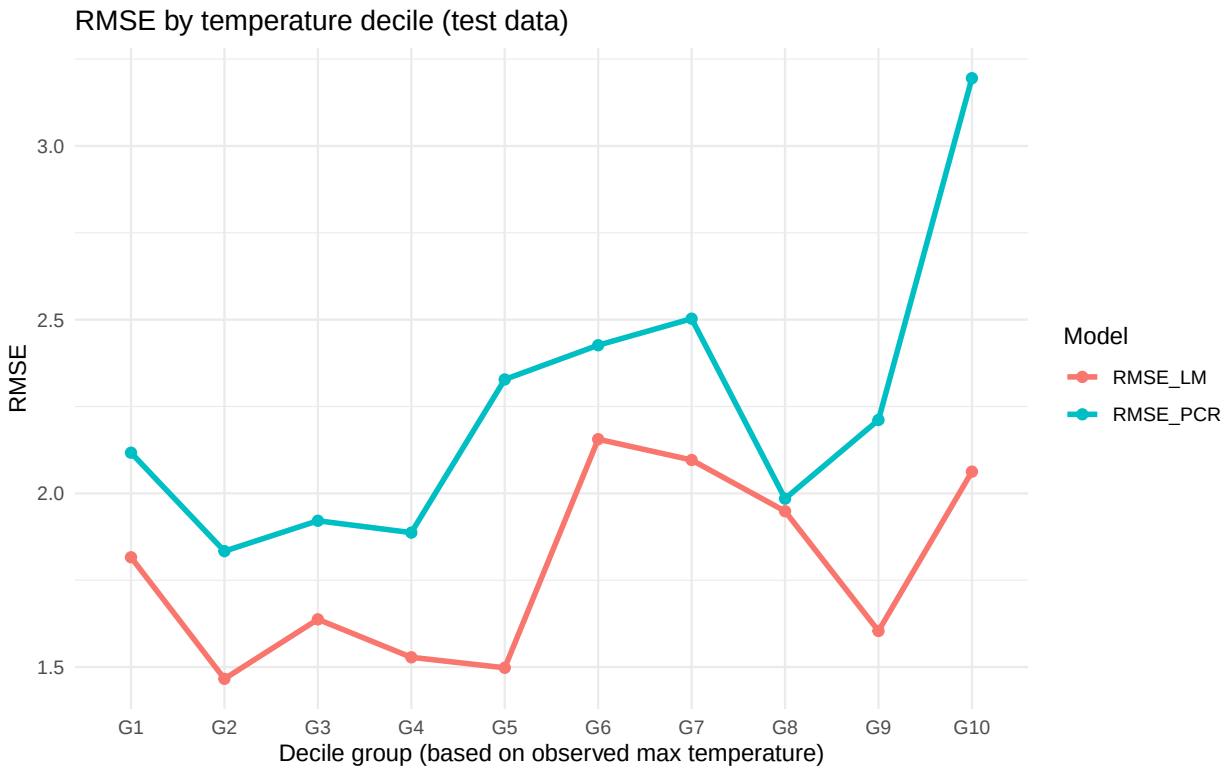



Table 6 presents the results of our Principal Component Regression (PCR) on the training set. Cross-validated RMSEP drops from 2.31 to 2.24, and finally to 2.06 when moving from 1 to 3 components, and changes only marginally at 4 components (2.05), indicating diminishing returns beyond k = 3. As a benchmark, we fit a standard multiple linear regression (OLS) to the original predictors. On the held-out test data, OLS achieves a lower RMSE (1.80) than PCR with k = 3 (2.16). PCR's $R^2$ value is high on both train and test datasets, but the absolute error is slightly larger than OLS in this split. This suggests that, for this horizon and feature set, compressing predictors with unsupervised PCA does not by itself improve point prediction accuracy over a well-specified linear model. This is consistent with expectations given (1) the near-linear relations between thermal and radiative predictors and next-day maxima and (2) inclusion of same-day max_temperature_c as a strong lagged signal that supervised OLS can exploit directly, whereas unsupervised PCA is not optimized for the target.




Because PCA optimizes total variance, not tail loss, it can under-weight rare extremes even if those are operationally important. That limitation motivates our final check: grouping test observations into deciles by realized next-day heat and plotting RMSE by method. The resulting curves are broadly similar across deciles (error does not spike dramatically in specific bins for this split), with OLS generally at or below PCR. Error profiles are not strongly dependent on the heat level in this split; if tail fidelity becomes a priority, one could consider quantile or weighted regression, EVT-informed losses, or nonlinear terms (e.g., splines for radiation or seasonality).




## Conclusion and Discussion

PCA successfully compressed the weather feature space into three interpretable dimensions that together explain ~82% of training variance. The retained components capture a warm–sunny–dry vs cool–overcast–wet gradient (PC1), a precipitation–gustiness axis (PC2), and wind strength vs warmth (PC3). However, when evaluated out-of-sample on a contiguous 20% test set, the OLS model outperforms the PCA, with an RSME ( 1.80) lower than PCR ( 2.16). Sensitivity checks showed diminishing returns beyond 3 principal components, aligning with the scree/parallel-analysis decision rule. Answering the central research question, the study finds that PCA-based feature extraction does not improve next day maximum temperature prediction over a well-specified linear regression, for this specific horizon, city (Rome), and split. However, PCA remains valuable for diagnostics, de-correlation, and compact reporting, but not as a stand-alone route to lower point-forecast error here.

Two design choices likely shaped this outcome and point to refinements. First, PCA is unsupervised and it maximizes total variance rather than temperature predictive variance. Supervised alternatives like OLS may better exploit signal under collinearity. Under collinearity, ridge/elastic-net would also be expected to match or exceed PCR by targeting predictive variance directly while keeping all (ridge) or grouped (elastic-net) signals. Second, two features merit targeted treatment: the inclusion of same-day `max_temperature_c` as a lagged regressor- useful but potentially dominating simpler components- and circular wind direction, which was included untransformed. Encoding direction via sin / cos terms can make wind-related structure legible to linear methods. For robustness, future work should use rolling-origin evaluation (rather than a single 80/20 split), probe nonlinearities/interactions (e.g., splines for radiation/seasonality), and re-test decile performance with an emphasis on extremes.

## Appendix A

Table 1: Correlations with Next-day Maximum Temperature

| Variable | Pearson $r$ |
|---|---|
| max_temperature_c | 0.969 |
| perceived_max_temperature_c | 0.963 |
| mean_temperature_c | 0.956 |
| perceived_mean_temperature_c | 0.950 |
| perceived_min_temperature_c | 0.906 |
| min_temperature_c | 0.903 |
| reference_evapotranspiration_mm | 0.870 |
| daylight_duration_s | 0.779 |
| shortwave_radiation_sum_mj_m2 | 0.769 |
| sunshine_duration_s | 0.649 |
| dominant_wind_direction | 0.434 |
| max_wind_gusts_km_h | 0.120 |
| max_wind_speed_km_h | 0.005 |
| snowfall_sum_mm | −0.086 |
| rain_sum_mm | −0.190 |
| precipitation_sum_mm | −0.195 |
| precipitation_hours_h | −0.300 |

Table 2: PCA Eigenvalues (Training Set)

| PC | Eigenvalue |
|---|---|
| PC1 | 8.825 |
| PC2 | 3.464 |
| PC3 | 1.585 |
| PC4 | 1.004 |
| PC5 | 0.890 |
| PC6 | 0.828 |
| PC7 | 0.547 |
| PC8 | 0.387 |
| PC9–PC17 | $< 0.31$ |

Table 3: Variance Explained by Principal Components (Training Set)

| PC | Proportion of Variance | Cumulative Variance |
|---|---|---|
| PC1 | 0.519 | 0.519 |
| PC2 | 0.203 | 0.723 |
| PC3 | 0.093 | 0.816 |
| PC4 | 0.059 | 0.875 |
| PC5 | 0.046 | 0.922 |
| PC6 | 0.040 | 0.962 |
| PC7 | 0.018 | 0.980 |
| PC8 | 0.008 | 0.988 |
| PC9–PC17 | $\approx 0.012$ (total) | 1.000 |

Table 4: Parallel Analysis (Training): Real Eigenvalues vs. 95% Cutoffs

| PC | Real Eigenvalue | 95% Cutoff | Keep |
|---|---|---|---|
| PC1 | 8.825 | ≈1.1 | Yes |
| PC2 | 3.464 | ≈1.1 | Yes |
| PC3 | 1.585 | ≈1.1 | Yes |
| PC4 | 1.004 | ≈1.1 | |
| PC5+ | $< 1$ | ≈1.1 | |

Table 5: PCA Loadings (PC1–PC3, Training Set)

| Variable | PC1 | PC2 | PC3 |
|---|---|---|---|
| mean_temperature_c | −0.32 | −0.10 | 0.13 |
| max_temperature_c | −0.33 | −0.04 | 0.10 |
| min_temperature_c | −0.30 | −0.16 | 0.17 |
| perceived_mean_temperature_c | −0.32 | −0.09 | 0.19 |
| perceived_max_temperature_c | −0.32 | −0.04 | 0.16 |
| perceived_min_temperature_c | −0.30 | −0.14 | 0.21 |
| max_wind_speed_km_h | 0.01 | −0.35 | −0.56 |
| max_wind_gusts_km_h | −0.03 | −0.38 | −0.52 |
| shortwave_radiation_sum_mj_m2 | −0.30 | 0.09 | −0.20 |
| dominant_wind_direction | −0.17 | −0.10 | −0.13 |
| reference_evapotranspiration_mm | −0.32 | 0.02 | −0.18 |
| daylight_duration_s | −0.29 | −0.06 | −0.13 |
| sunshine_duration_s | −0.26 | 0.20 | −0.21 |
| precipitation_sum_mm | 0.09 | −0.46 | 0.20 |
| snowfall_sum_mm | 0.03 | −0.03 | −0.08 |
| precipitation_hours_h | 0.12 | −0.43 | 0.16 |
| rain_sum_mm | 0.09 | −0.46 | 0.21 |

Table 6: PCR Cross-Validated RMSEP by Number of Components (Training)

| $k$ | RMSEP (CV) |
|---|---|
| 1 | 2.305 |
| 2 | 2.244 |
| 3 | 2.055 |
| 4 | 2.052 |

Table 7: Test Performance: OLS vs. PCR ($k = 3$)

| Model | RMSE (Test) | $R^2$ (Train) | $R^2$ (Test) |
|---|---|---|---|
| OLS (All Variables) | 1.800 | — | — |
| PCR ($k = 3$) | 2.156 | 0.920 | 0.925 |

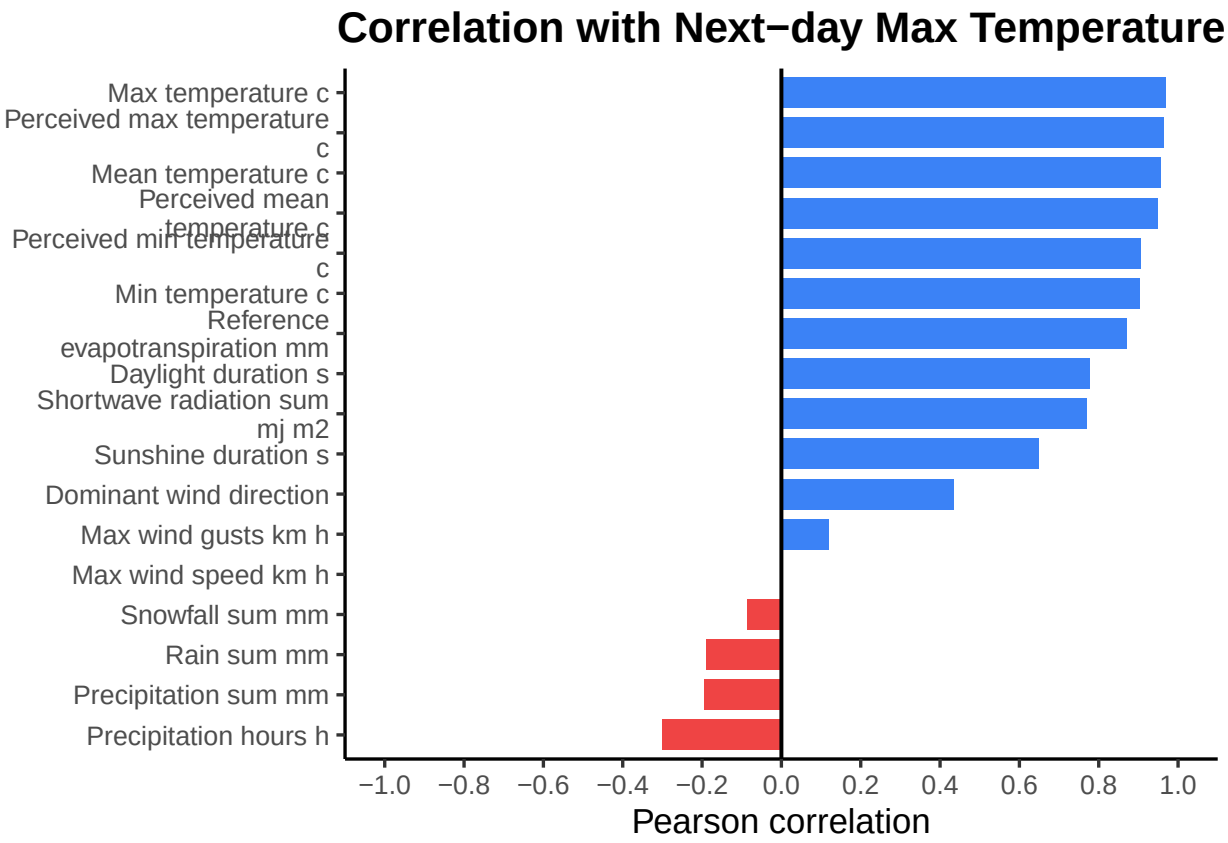
Table 8: RMSE by Observed Max-Temperature Decile (Test Set)

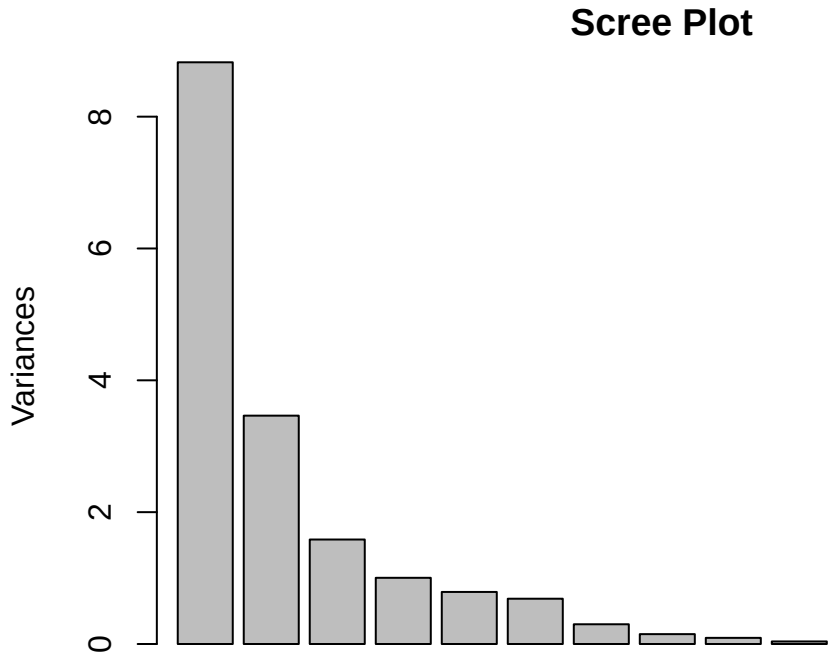
| Decile Group | RMSE: OLS | RMSE: PCR ($k = 3$) |
|---|---|---|
| G1 (coolest) | | |
| G2 | | |
| G3 | | |
| G4 | | |
| G5 | | |
| G6 | | |
| G7 | | |
| G8 | | |
| G9 | | |
| G10 (hottest) | | |

## Appendix B



Figure 1: Correlation Scatter Plots


Correlation with Next−day Max Temperature
Max temperature c
Perceived max temperature c
Mean temperature c
Perceived mean temperature c
Perceived min temperature c
Min temperature c
Reference evapotranspiration mm
Daylight duration s
Shortwave radiation sum mj m2
Sunshine duration s
Dominant wind direction
Max wind gusts km h
Max wind speed km h
Snowfall sum mm
Rain sum mm
Precipitation sum mm
Precipitation hours h
−1.0
−0.8
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
Pearson correlation


Scree Plot
Variances
0
2
4
6
8

## Appendix C

```
## # Appendix C. Full code

## ```r

##  knitr::opts_chunk$set(echo=FALSE, message=FALSE, warning=FALSE)
## library(readr)
## library(tidyverse)
## library(janitor)
## library(ggplot2)
## library(dplyr)
## library(stringr)
## rm(list = ls())
## # Directory setup
## #path = dirname(rstudioapi::getSourceEditorContext()$path) # Path is directory of this file
## #setwd(path)
## # no scientific notations
## options(scipen = 999)
## data <- read.csv("a2_data_group_9.csv")
## names(data)
##
## # Preprocessing
## data <- janitor::clean_names(data) # cleans all the cols names automatically
## names(data)
##
## data <- data %>%
##   select(-location_id)
## # --- 1. Create X and y ---
##
## # Build the X matrix: all variables, except the last row
## X <- as.matrix(data[-nrow(data), ]) # this includes the date col
##
## # Build the y vector: the max temperature column, except its first observation
## y <- data$max_temperature_c[-1]
##
## # Check alignment and dimensions
## dim(X)  # should be (n-1) x p
## length(y)  # should be (n-1)
## # --- 2. Compute correlations ---
##
## # 0) Ensure all-numeric predictors and aligned X/y
## df_corr <- data %>% dplyr::select(where(is.numeric))
##
## X_corr <- df_corr[-nrow(df_corr), ]            # data.frame (predictors at time t)
## y_corr <- df_corr$max_temperature_c[-1]        # vector (target at time t+1)
##
## # 1) Correlations
## correlations <- sapply(X_corr, function(x) cor(x, y_corr, use = "complete.obs"))
## correlations <- sort(correlations, decreasing = TRUE)
## print(correlations)
##
## # 2) Plot ALL variables
## num_vars <- ncol(X_corr)
```

```
## # par(mfrow = c(4, 5))   # 4 rows × 5 columns grid (enough for 17 plots)
## #
## # for (col in names(correlations)) {
## #   x <- X_corr[[col]]
## #   plot(x, y_corr,
## #        main = paste("M vs", col),
## #        xlab = col,
## #        ylab = "Next-day (°C)",
## #        pch = 19, col = "darkblue")
## #   abline(lm(y_corr ~ x), col = "red", lwd = 2)
## # }
## #
## # par(mfrow = c(1, 1))  # reset plotting layout
## # 3) Correlation summary bar chart for the report
##
## # correlations should already be a named numeric vector
## corr_df <- tibble(
##   variable = names(correlations),
##   corr = as.numeric(correlations)
## ) %>%
##   arrange(desc(corr)) %>%  # positives first, then negatives
##   mutate(
##     label = str_replace_all(variable, "_", " "),
##     label = str_to_sentence(label),
##     label = str_wrap(label, width = 25),
##     label = factor(label, levels = rev(label))  # keep sorted order
##   )
##
## # # Plot
## # ggplot(corr_df, aes(x = label, y = corr, fill = corr > 0)) +
## #   geom_col(width = 0.75) +
## #   geom_hline(yintercept = 0, color = "black", linewidth = 0.7) +
## #   coord_flip() +
## #   labs(
## #     title = "Correlation with Next-day Max Temperature",
## #     x = NULL,
## #     y = "Pearson correlation"
## #   ) +
## #   scale_fill_manual(values = c("TRUE" = "#3B82F6", "FALSE" = "#EF4444")) +
## #   scale_y_continuous(
## #     limits = c(-1, 1),
## #     breaks = seq(-1, 1, 0.2)
## #   ) +
## #   theme_minimal(base_size = 13) +
## #   theme(
## #     legend.position = "none",      # remove legend
## #     panel.grid.major.y = element_blank(),
## #     panel.grid.minor = element_blank(),
## #     plot.title = element_text(face = "bold", hjust = 0.5),
## #     axis.text.y = element_text(size = 10)
## #   )
## # --- 3. Train Test Split (Time Series) ---
##
## # 0) Ensure time order
```

```
## data <- data %>% arrange(date)
##
## # 1) Keep only numeric predictors (this automatically drops Date)
## X_df <- data %>% select(where(is.numeric))  # includes max_temperature_c
##
## # 2) Build aligned X (t) and y (t+1)
## X <- as.matrix(X_df[-nrow(X_df), , drop = FALSE])
## y <- data$max_temperature_c[-1]
##
## # 3) Time indices (keep separately; do NOT include in X)
## time_X <- data$date[-nrow(data)]
## time_y <- data$date[-1]
##
## # --- train/test split by proportion, no leakage ---
## n <- nrow(X); k <- floor(0.8 * n)
## X_train <- X[1:k, , drop = FALSE]; y_train <- y[1:k]
## X_test  <- X[(k+1):n, , drop = FALSE]; y_test <- y[(k+1):n]
## # --- 4. Generate PC on X_train ---
##
## # 1. Perform PCA *only* on training data
## pca_model <- prcomp(X_train, center = TRUE, scale. = TRUE)
##
## # 2. Check how much variance each component explains
## summary(pca_model)
##
## # 3. Look at the contribution of each variable to each PC
## round(pca_model$rotation,2)
## # 2. Eigenvalues (variances of PCs) and explained variance
## eig  <- pca_model$sdev^2
##
## # Show only eigenvalues > 1 (Kaiser's rule)
## data.frame(
##   PC = paste0("PC", seq_along(eig)),
##   Eigenvalue = eig
## ) %>%
##   dplyr::filter(Eigenvalue > 1)
##
## # 3. Using Cumulative VAF
## prop_var <- eig / sum(eig)
## cum_var  <- cumsum(prop_var)
## tau   <- 0.85
## k_vaf <- which(cum_var >= tau)[1]
## k_vaf
##
## cum_var
## # 4
## source("permtestPCA.R")          # Load the permtestPCA() function
## perm_range <- permtestPCA(X_train)
##
## dev.new(width = 8, height = 5)
##
## # --- Permutation (Parallel Analysis) for choosing number of PCs ---
##
## # X_train: numeric matrix/data.frame (observations x variables)
```

```
## # B: number of permutations (e.g., 1000)
## # alpha: significance level for the cutoff (0.05 uses 95th percentile of permuted eigs)
## # Returns a list with suggested k and helpful objects, and draws a scree-style plot.
## perm_parallel_pca <- function(X_train, B = 1000, alpha = 0.05, seed = 42,
##                               center = TRUE, scale. = TRUE, make_plot = TRUE) {
##   stopifnot(is.data.frame(X_train) || is.matrix(X_train))
##   if (!is.null(seed)) set.seed(seed)
##
##   X <- as.matrix(X_train)
##   n <- nrow(X)
##   p <- ncol(X)
##
##   # 1) PCA on the real data
##   pca_real <- prcomp(X, center = center, scale. = scale.)
##   eig_real <- pca_real$sdev^2  # length p
##
##   # 2) Permutation: shuffle rows within each column to break correlation, keep marginals
##   perm_eigs <- replicate(B, {
##     Xb <- apply(X, 2, function(col) sample(col, size = n, replace = FALSE))
##     # PCA on permuted data
##     pb <- prcomp(Xb, center = center, scale. = scale.)
##     pb$sdev^2
##   })
##
##   perm_eigs <- t(perm_eigs)  # B x p (rows=replicates)
##
##   # 3) For each component j, get the (1-alpha) quantile across permutations
##   q_perm <- apply(perm_eigs, 2, quantile, probs = 1 - alpha, names = FALSE)
##
##   # 4) Suggested k: how many components have real eigenvalue > permutation cutoff
##   keep_vec <- eig_real > q_perm
##   k_suggested <- if (any(keep_vec)) max(which(keep_vec)) else 0
##
##   # 5) Helpful summaries
##   vaf_real <- eig_real / sum(eig_real)
##   cum_vaf_real <- cumsum(vaf_real)
##   vaf_q_perm <- q_perm / sum(eig_real)        # put cutoffs on same scale for plotting
##   cum_vaf_q_perm <- cumsum(vaf_q_perm)
##
##   # 6) Plot
##   if (make_plot) {
##     op <- par(no.readonly = TRUE); on.exit(par(op), add = TRUE)
##
##     # Scree with cutoff
##     plot(1:p, eig_real, type = "b", pch = 16,
##          xlab = "Principal component", ylab = "Eigenvalue",
##          main = sprintf("Parallel Analysis (Permutation): suggested k = %d", k_suggested))
##     lines(1:p, q_perm, type = "b", pch = 1)
##     abline(v = k_suggested + 0.5, lty = 3)  # visual separator after chosen k
##     legend("topright",
##            legend = c("Real data eigenvalues", sprintf("Permutation cutoff (%.0f%%)", (1 - alpha) * 1
##            pch = c(16, 1), lty = 1, bty = "n")
##   }
##
```

```
##   list(
##     k_suggested = k_suggested,
##     eigen_real = eig_real,
##     eigen_perm = perm_eigs,   # B x p matrix
##     cutoff_quantile = q_perm, # length p (eigenvalue thresholds)
##     keep = keep_vec,          # logical vector of length p
##     vaf_real = vaf_real,
##     cum_vaf_real = cum_vaf_real
##   )
## }
##
## perm_range <- perm_parallel_pca(X_train)
## # --- 7. 2 Construct the biplots ---
##
## # Biplot of first 2 PCs
## biplot(pca_model, scale = 0)
##
## library(factoextra)
## library(ggplot2)
## library(patchwork)
##
## # --- If your dataset is huge, optionally downsample *for plotting only* ---
## set.seed(1)
## plot_idx <- seq_len(min(4000, nrow(X_train)))  # or sample.int(nrow(X_train), 4000)
## pca_plot <- prcomp(X_train[plot_idx, , drop = FALSE], center = TRUE, scale. = TRUE)
##
## # A. PC1 vs PC2
## p12 <- fviz_pca_biplot(
##   pca_plot,
##   axes = c(1, 2),
##   label = "var",           # only label variables
##   repel = TRUE,             # avoid overlap
##   col.var = "#C43E3E",     # red loadings
##   arrowsize = 0.7,
##   col.ind = "skyblue3",    # points
##   alpha.ind = 0.15,         # transparency
##   pointsize = 0.6
## ) +
##   coord_fixed() +
##   theme_minimal(base_size = 12) +
##   theme(
##     panel.grid.minor = element_blank(),
##     legend.position = "none"
##   ) +
##   labs(title = "Biplot Components 1 and 2", x = "Comp.1", y = "Comp.2")
## p12
##
## # B. PC2 vs PC3
## p23 <- fviz_pca_biplot(
##   pca_plot,
##   axes = c(2, 3),
##   label = "var",
##   repel = TRUE,
##   col.var = "#C43E3E",
```

```
##   arrowsize = 0.7,
##   col.ind = "skyblue3",
##   alpha.ind = 0.15,
##   pointsize = 0.6
## ) +
##   coord_fixed() +
##   theme_minimal(base_size = 12) +
##   theme(
##     panel.grid.minor = element_blank(),
##     legend.position = "none"
##   ) +
##   labs(title = "Biplot Components 2 and 3", x = "Comp.1", y = "Comp.2")
##
## # Side-by-side layout
## p12 + p23
##
## # Loadings
## loadings <- pca_model$rotation
## round(loadings, 2)
##
## # Optionally visualize
## fviz_pca_biplot(pca_model)
## # --- 8. Bootstrap Confidence Interval for choosen number of PCs ---
##
## set.seed(42)
##
## # Assumes you already have X_train (numeric matrix/data.frame of predictors only)
## k <- 3
##
## # Fit PCA once on the original training set (useful for reporting point estimate)
## pca_train <- prcomp(X_train, center = TRUE, scale. = TRUE)
## eig_train <- pca_train$sdev^2
## vaf_k_hat <- sum(eig_train[1:k]) / sum(eig_train)   # point estimate
##
## # Bootstrap (simple percentile CI)
## B <- 1000
## vaf_boot <- replicate(B, {
##   idx <- sample.int(nrow(X_train), size = nrow(X_train), replace = TRUE)
##   Xb  <- X_train[idx, , drop = FALSE]
##   pca_b <- prcomp(Xb, center = TRUE, scale. = TRUE)
##   eig_b <- pca_b$sdev^2
##   sum(eig_b[1:k]) / sum(eig_b)
## })
##
## ci <- quantile(vaf_boot, c(0.025, 0.975))
## list(
##   point_estimate = vaf_k_hat,
##   ci_95 = ci,
##   mean_boot = mean(vaf_boot),
##   sd_boot = sd(vaf_boot)
## )
##
## # Convert to data frame for ggplot
## df_boot <- data.frame(vaf = vaf_boot)
```

```
##
## # Plot density + CI + point estimate
## ggplot(df_boot, aes(x = vaf)) +
##   geom_histogram(aes(y = ..density..),
##                  bins = 40, fill = "skyblue3", color = "white", alpha = 0.6) +
##   geom_density(color = "darkblue", linewidth = 1) +
##   geom_vline(xintercept = vaf_k_hat, color = "red", linetype = "solid", linewidth = 1) +
##   geom_vline(xintercept = ci[1], color = "darkred", linetype = "dashed", linewidth = 1) +
##   geom_vline(xintercept = ci[2], color = "darkred", linetype = "dashed", linewidth = 1) +
##   labs(
##     title = "Bootstrap distribution of total variance explained (first 4 PCs)",
##     x = "Total variance explained",
##     y = "Density",
##     subtitle = sprintf("Red line = point estimate (%.2f%%)\nDashed = 95%% CI [%.2f%%, %.2f%%]",
##                        100*vaf_k_hat, 100*ci[1], 100*ci[2])
##   ) +
##   theme_minimal(base_size = 13)
## #####
## # Install/load boot if needed
## if (!requireNamespace("boot", quietly = TRUE)) install.packages("boot")
## library(boot)
##
## set.seed(42)
##
## # Inputs you already have:
## # X_train: numeric matrix/data.frame of predictors
## k <- 3
## B <- 1000
##
## # 1) Define a statistic function that returns ALL eigenvalues
## #    (just like your professor's example)
## eig_stat <- function(data, indices) {
##   Xb <- data[indices, , drop = FALSE]
##   pc <- prcomp(Xb, center = TRUE, scale. = TRUE)        # analogous to center=TRUE, scale.=TRUE
##   pc$sdev^2                                # return eigenvalues
## }
##
## # 2) Run the bootstrap
## fit.boot  <- boot(data = X_train, statistic = eig_stat, R = B)
##
## # 3) Extract the R x p matrix of eigenvalues
## eigs.boot <- fit.boot$t  # rows = bootstrap replicates, cols = eigenvalues
##
## # 4) Convert those eigenvalues to VAF_k for each bootstrap replicate
## vaf_boot <- apply(eigs.boot, 1, function(ev) sum(ev[1:k]) / sum(ev))
##
## # 5) Point estimate via the same pipeline on the original sample
## pc0 <- princomp(X_train, cor = TRUE)
## eig0 <- pc0$sdev^2
## vaf_k_hat <- sum(eig0[1:k]) / sum(eig0)
##
## # 6) CI (percentile, to match your current approach)
## ci <- quantile(vaf_boot, c(0.025, 0.975))
##
```

```
## # 7) Summary output
## summary_list <- list(
##   point_estimate = vaf_k_hat,
##   ci_95 = ci,
##   mean_boot = mean(vaf_boot),
##   sd_boot = sd(vaf_boot)
## )
## print(summary_list)
##
## # 8) Plot the bootstrap distribution
## hist(vaf_boot,
##      breaks = 30,
##      main = sprintf("Bootstrap Distribution of VAF for First %d PCs", k),
##      xlab = "VAF (Variance Accounted For)",
##      col = "skyblue", border = "white")
## abline(v = vaf_k_hat, col = "red", lwd = 2, lty = 2)
## abline(v = ci, col = "darkgreen", lwd = 2, lty = 3)
## legend("topright", legend = c("Point Estimate", "95% CI"),
##        col = c("red", "darkgreen"), lty = c(2, 3), bty = "n")
##
## ####
##
## # --- 9. Fit the choosen PCs (k) -----
##
## if (!requireNamespace("pls", quietly = TRUE)) install.packages("pls")
## library(pls)
##
## set.seed(42)
##
## k <- k
##
## # Fit PCR with chosen number of components
## pcr_fit <- pcr(
##   y_train ~ .,
##   data = data.frame(y_train = y_train, X_train),
##   scale = TRUE,
##   center = TRUE,
##   validation = "CV",
##   ncomp = k   # <-- specify number of components to use
## )
##
## # Check model summary
## summary(pcr_fit)
##
## # --- 10. Fit a benchmark MLR -----
##
## # Fit a standard multiple linear regression (no dimensionality reduction)
## lm_fit <- lm(y_train ~ ., data = data.frame(y_train = y_train, X_train))
##
## # Check model summary
## summary(lm_fit)
##
## # PCR predictions (specify number of components = 3)
## pcr_pred_test <- predict(pcr_fit, newdata = data.frame(X_test), ncomp = 3)
```

```
##
## # MLR predictions
## lm_pred_test <- predict(lm_fit, newdata = data.frame(X_test))
##
## # --- 11. Performance metrics -----
##
## # Define RMSE function
## rmse <- function(actual, predicted) {
##   sqrt(mean((actual - predicted)^2))
## }
##
## # Calculate RMSE for test set
## lm_rmse_test  <- rmse(y_test, lm_pred_test)
## pcr_rmse_test <- rmse(y_test, pcr_pred_test)
##
## # Display results
## lm_rmse_test
## pcr_rmse_test
##
## # Compute R² for PCR train set
## pcr_pred_train <- predict(pcr_fit, newdata = data.frame(X_train), ncomp = 3)
## ss_res_train <- sum((y_train - pcr_pred_train)^2)
## ss_tot_train <- sum((y_train - mean(y_train))^2)
## pcr_r2_train <- 1 - (ss_res_train / ss_tot_train)
##
## pcr_r2_train
##
## # Compute R² for PCR test set
## ss_res <- sum((y_test - pcr_pred_test)^2)
## ss_tot <- sum((y_test - mean(y_test))^2)
## pcr_r2_test <- 1 - (ss_res / ss_tot)
##
## pcr_r2_test
##
## # --- 12. k + 1 and k - 1 -----
##
## # Fit PCR with chosen number of components + 1 (k + 1)
## pcr_fit1 <- pcr(
##   y_train ~ .,
##   data = data.frame(y_train = y_train, X_train),
##   scale = TRUE,
##   center = TRUE,
##   validation = "CV",
##   ncomp = k + 1   # <-- specify number of components to use
## )
##
## summary(pcr_fit1)
##
## # PCR predictions
## pcr_pred_test <- predict(pcr_fit1, newdata = data.frame(X_test), ncomp = k + 1)
##
## # Fit PCR with chosen number of components - 1 (k - 1)
## pcr_fit2 <- pcr(
##   y_train ~ .,
```

```
##   data = data.frame(y_train = y_train, X_train),
##   scale = TRUE,
##   center = TRUE,
##   validation = "CV",
##   ncomp = k - 1   # <-- specify number of components to use
## )
##
## summary(pcr_fit2)
##
## # PCR predictions
## pcr_pred_test <- predict(pcr_fit2, newdata = data.frame(X_test), ncomp = k - 1)
## # --- 13 -----
##
## # Combine observed and predicted values
## results <- data.frame(
##   y_test = y_test,
##   lm_pred = lm_pred_test,
##   pcr_pred = as.numeric(pcr_pred_test)
## )
##
## # Create decile groups based on observed y_test values
## results$group <- cut(
##   results$y_test,
##   breaks = quantile(results$y_test, probs = seq(0, 1, 0.1)),
##   include.lowest = TRUE,
##   labels = paste0("G", 1:10)
## )
##
## rmse_by_group <- results %>%
##   group_by(group) %>%
##   summarise(
##     RMSE_LM  = rmse(y_test, lm_pred),
##     RMSE_PCR = rmse(y_test, pcr_pred)
##   )
##
## # Convert to long format for easier plotting
## rmse_long <- rmse_by_group %>%
##   tidyr::pivot_longer(cols = c(RMSE_LM, RMSE_PCR),
##                       names_to = "Model",
##                       values_to = "RMSE")
##
## # Plot
## ggplot(rmse_long, aes(x = group, y = RMSE, color = Model, group = Model)) +
##   geom_line(size = 1.2) +
##   geom_point(size = 2) +
##   theme_minimal() +
##   labs(
##     title = "RMSE by temperature decile (test data)",
##     x = "Decile group (based on observed max temperature)",
##     y = "RMSE",
##     color = "Model"
##   )
## # local({
## #   op <- par(no.readonly = TRUE); on.exit(par(op), add = TRUE)
```

```
## #
## #   par(mfrow = c(6, 3),
## #       mar = c(3, 3, 3, 1),
## #       oma = c(0, 0, 0, 0),     # outer margins a 0
## #       mgp = c(1.3, 0.4, 0))    # distancia de ejes/labels
## #
## #   for (col in names(correlations)) {
## #     x <- X_corr[[col]]
## #     y <- y_corr
## #     ok <- is.finite(x) & is.finite(y); x <- x[ok]; y <- y[ok]
## #
## #     plot(x, y,
## #          main = paste("Next-day Max Temp vs", col),
## #          xlab = col, ylab = "Next-day Max Temp (°C)",
## #          pch = 16, cex = 0.5, col = rgb(0,0,0.55,0.25))
## #     abline(lm(y ~ x), col = rgb(0.8,0,0,0.9), lwd = 1.4)
## #   }
## # })
##
## knitr::include_graphics("scatterplot.png")
## # Plot
## ggplot(corr_df, aes(x = label, y = corr, fill = corr > 0)) +
##   geom_col(width = 0.75) +
##   geom_hline(yintercept = 0, color = "black", linewidth = 0.7) +
##   coord_flip() +
##   labs(
##     title = "Correlation with Next-day Max Temperature",
##     x = NULL,
##     y = "Pearson correlation"
##   ) +
##   scale_fill_manual(values = c("TRUE" = "#3B82F6", "FALSE" = "#EF4444")) +
##   scale_y_continuous(
##     limits = c(-1, 1),
##     breaks = seq(-1, 1, 0.2)
##   ) +
##   theme_classic(base_size = 13) +
##   theme(
##     legend.position = "none",      # remove legend
##     panel.grid.major.y = element_blank(),
##     panel.grid.minor = element_blank(),
##     plot.title = element_text(face = "bold", hjust = 0.5),
##     axis.text.y = element_text(size = 10)
##   )
## # --- 6. 2 methods to find the the optimal number of PC ---
##
## # 1. Visualize variance explained
## op <- par(mar = c(5, 5, 2, 1) + 0.1)           # bigger margins: bottom, left, top, right
## plot(pca_model, type = "b", main = "Scree Plot",
##      xlim = c(0.5, length(pca_model$sdev) + 0.5))  # pad the ends so bars/points aren't clipped
## par(op)
## # Extract ONLY the code from R chunks in this Rmd and print it as one block
## lines <- readLines(knitr::current_input(), warn = FALSE)
##
## r_code <- character(0)
```

```
## open <- FALSE
## for (ln in lines) {
##   if (grepl("^```\\{r( |\\}|$)", ln)) {        # start of an R chunk
##     open <- TRUE
##     next
##   }
##   if (open && grepl("^```\\s*$", ln)) {        # end of a chunk
##     open <- FALSE
##     next
##   }
##   if (open) r_code <- c(r_code, ln)            # keep only lines inside R chunks
## }
##
## cat("# Appendix C. Full code\n\n")
## cat("```r\n")
## cat(paste(r_code, collapse = "\n"))
## cat("\n```\n")

##
## ```
```