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1  # =====
2  # TEİAŞ DGP 0-1 – FINAL PIPELINE (Multi-State + Hankel + AFFINE DMD/DMDc)
3  # FULL MERGED VERSION (RUN ONCE) – EXTENDED (Excel matrix exports + RF/LR comparison)
4  #
5  # ☒ Two preprocessing modes:
6  #     (A) Pipeline 1..9 FULL (Original/Long/6h/Norm/WideByDate)
7  #     (B) TPYS FAST + (loglp -> MinMax row-wise)
8  #
9  # ☒ Affine DMD:  $x^* = A x + b$ 
10 # ☒ Affine DMDc:  $x^* = A x + B u + b$ 
11 # ☒ Hankel-Affine versions
12 # ☒ Optional spike hybrid correction (in-sample)
13 #
14 # ☒ Exports to Excel (each in its own sheet):
15 #     - X_real, X1, X2
16 #     - A, b (+ Hankel Ah, bh)
17 #     - DMD: Xaffine_dmd (Xdmd), Xaffine_dmd_hankel (Xhan)
18 #     - DMDc: Xaffine_dmdc (Xrec), Xaffine_dmdc_hankel (Xh)
19 #     - Normalized versions (0..1): Xn, Xdmd_n, Xhan_n, Un, Xrec_n, Xh_n
20 #
21 # ☒ NEW (YOU REQUESTED):
22 #     1) Read/keep matrices: X_real, X1, X2, A, B, Xaffine outputs
23 #         and export them to RESULTS_ALL.xlsx each in its own sheet.
24 #     2) RF & LR ML comparison (1-year horizon):
25 #         - Train on earlier part, test on last "year" samples
26 #         - Plot "Real vs Pred" + "Error curve" for RF and LR
27 #         - Performance evaluation + graphical analysis
28 #
29 # IMPORTANT REQUIREMENT (YOUR NOTE):
30 #     Hankel outputs MUST NOT have negative values and should be in [0, 1].
31 #     Therefore: we apply Hankel only on normalized matrices, then clip to [0,1]
32 #     before saving / returning.
33 # =====
34
35 import os
36 import itertools
37 import numpy as np
38 import pandas as pd
39
40 import matplotlib
41 matplotlib.use("Agg")
42 import matplotlib.pyplot as plt
43
44 from numpy.linalg import svd
45
46 # -----
47 # 0) PATHS & FLAGS
48 # -----
49 DATA_DIR = r"C:\Users\OMER\new dmd tias kodlarım" # [P01] Workspace folder path
50           (change if your files moved)
51 XLSX_NAME = "DGP_0-1_Kodlu_Talimat_Hacimleri_regime6h_NORMALIZED.xlsx" # [P02] Input
52           Excel filename
53 XLSX_PATH = os.path.join(DATA_DIR, XLSX_NAME)
54
55 TPYS_SHEET = "TPYS" # [P03] Sheet name containing TPYS data
56
57 # =====
58 # (NEW) Choose ONE preprocessing mode
59 # =====
60 USE_PIPELINE_1_9 = True # [P04] True => Pipeline 1..9 FULL
61 USE_TPYS_FAST = False # [P05] True => TPYS FAST + loglp->MinMax row-wise
62
63 if USE_PIPELINE_1_9 == USE_TPYS_FAST:
64     raise ValueError("Choose exactly ONE preprocessing mode: set
65                       USE_PIPELINE_1_9=True and USE_TPYS_FAST=False (or vice versa).")
66
67 DO_CLEAN_NORMALIZE = True # [P06] True => run preprocessing (clean/normalize).
68                           False => only read wide
69
70 # Output for pipeline 1..9 workbook
71 PIPELINE_1_9_OUT_NAME = "PIPELINE_6H_PREPROCESS.xlsx" # [P07] Output Excel for steps

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1..9
68 PIPELINE_1_9_OUT_PATH = os.path.join(DATA_DIR, PIPELINE_1_9_OUT_NAME)
69
70 # Output for TPYS fast processed wide
71 PROCESSED_WIDE_NAME = "TPYS_WIDE_PROCESSED.xlsx" # [P08] Wide output for fast path
72 PROCESSED_WIDE_PATH = os.path.join(DATA_DIR, PROCESSED_WIDE_NAME)
73 PROCESSED_WIDE_SHEET = "WIDE" # [P09] Sheet name inside the processed wide file
74
75 OUT_XLSX = os.path.join(DATA_DIR, "RESULTS_ALL.xlsx") # [P10] Final results Excel
76 FIG_ROOT = os.path.join(DATA_DIR, "RESULTS_FIGS") # [P11] Figures output folder
77
78 CALIBRATION_MODE = "auto" # [P12] "manual" or "auto" (Grid Search)
79
80 SAVE_PLOTS = True # [P13] Save plots to disk
81 PLOT_STEP_3D = 4 # [P14] Sampling step for 3D surfaces
82
83 # -----
84 # (NEW) AFFINE + SPIKES OPTIONS
85 # -----
86 USE_AFFINE_MODELS = True # [P15] Enable affine DMD/DMDc
87 USE_HANKEL_AFFINE = True # [P16] Enable Hankel-affine versions
88 USE_SPIKE_HYBRID = True # [P17] Spike correction (in-sample blending)
89 SPIKE_Q = 0.995 # [P18] Quantile over |diff| to detect spikes
90 SPIKE_BLEND = 0.85 # [P19] Blend ratio of real at spike indices
91
92 # -----
93 # 0.1) GRID CONTROL
94 # -----
95 MAX_TRIALS_DMD = 80 # [P20] Maximum grid trials for DMD
96 MAX_TRIALS_DMDc = 120 # [P21] Maximum grid trials for DMDc
97
98 PLOTS_DURING_GRID = False # [P22] If True, grid becomes slower due to plots
99
100 PATIENCE_DMD = 25 # [P23] Early stop patience for DMD grid
101 PATIENCE_DMDc = 35 # [P24] Early stop patience for DMDc grid
102
103 SMART_GRID = True # [P25] Enable stage-2 smart expansion
104 STAGE1_ONLY = False # [P26] If True, stop after stage-1
105 STAGE2_TOP_CANDIDATES = 2 # [P27] Expand around top K candidates
106 STAGE2_MULTIPLIERS_TIK = [0.5, 1.0, 2.0] # [P28] Tikhonov multipliers around best tik
107 STAGE2_NEIGHBOR_RANK = [-2, 0, +2] # [P29] Rank neighbors around best
108
109 # -----
110 # 1) Your column names in TPYS
111 # -----
112 DATE_COL = "Geçerlilik Tarihi" # [P30] Date column name in TPYS
113 HOUR_COL = "Saat" # [P31] Hour column name in TPYS
114
115 TPYS_COLS_REQUIRED = [
116     "Net Talimat",
117     "Yal 0 Miktar",
118     "Yal 1 Miktar",
119     "Yat 0 Miktar",
120     "Yat 1 Miktar",
121     "Yerine Getirilen YAL",
122     "Yerine Getirilen YAT",
123 ] # [P32] Required TPYS columns (update if your Excel changes)
124
125 # -----
126 # 2) Multi-State DMDc definition (EXACT)
127 # -----
128 STATE_ROWS = [
129     "Yerine Getirilen YAL",
130     "Yerine Getirilen YAT",
131     "Net Talimat",
132 ] # [P33] State rows used in DMDc
133
134 CONTROL_ROWS = [
135     "Yal 0 Miktar",
136     "Yal 1 Miktar",
137     "Yat 0 Miktar",

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138     "Yat 1 Miktar",
139 ] # [P34] Control rows used in DMDc
140
141 DMD_ROWS = STATE_ROWS[:,] # [P35] DMD rows for fair comparison (can change for
experiments)
142
143 # -----
144 # 3) MANUAL PARAMS (baseline)
145 # -----
146 MANUAL = dict(
147     # ---- DMD ----
148     DMD_RANK_MAX=40, # [P36]
149     DMD_TIK=1e-2, # [P37]
150     DMD_STABLE=True, # [P38]
151     DMD_RHO_MAX=0.995, # [P39]
152     DMD_CLIP=None, # [P40] Clip for rollout (None disables)
153
154     # Hankel-DMD
155     DMD_HANKEL_D=16, # [P41] Hankel window length d
156     DMD_HANKEL_RANK_MAX=120, # [P42]
157     DMD_HANKEL_TIK=1e-2, # [P43]
158     DMD_HANKEL_STABLE=True, # [P44]
159     DMD_HANKEL_RHO_MAX=0.995, # [P45]
160     DMD_HANKEL_CLIP=None, # [P46]
161
162     # ---- DMDc ----
163     DMDc_RANK_OMEGA=12, # [P47]
164     DMDc_TIK=1e-2, # [P48]
165     DMDc_STABLE=True, # [P49]
166     DMDc_RHO_MAX=0.995, # [P50]
167     DMDc_CLIP=None, # [P51]
168
169     # Hankel(DMDc)
170     DMDc_HANKEL_D=16, # [P52]
171     DMDc_HANKEL_RANK_MAX=120, # [P53]
172     DMDc_HANKEL_TIK=1e-2, # [P54]
173     DMDc_HANKEL_STABLE=True, # [P55]
174     DMDc_HANKEL_RHO_MAX=0.995, # [P56]
175     DMDc_HANKEL_CLIP=None, # [P57]
176 )
177
178 # -----
179 # 4) GRID SEARCH (Stage-1 safe)
180 # -----
181 GRID = dict(
182     # --- DMD + Hankel Stage-1 ---
183     DMD_RANK_GRID=[20, 40], # [P58]
184     DMD_TIK_GRID=[1e-2], # [P59]
185     DMD_RHO_MAX_GRID=[0.995], # [P60]
186     DMD_CLIP_GRID=[None], # [P61]
187
188     DMD_HANKEL_D_GRID=[16], # [P62]
189     DMD_HANKEL_RANK_GRID=[80, 120], # [P63]
190     DMD_HANKEL_TIK_GRID=[3e-2, 1e-2], # [P64]
191     DMD_HANKEL_RHO_MAX_GRID=[0.995], # [P65]
192     DMD_HANKEL_CLIP_GRID=[None], # [P66]
193
194     # --- DMDc + Hankel Stage-1 ---
195     DMDc_RANK_OMEGA_GRID=[10, 15], # [P67]
196     DMDc_TIK_GRID=[1e-2, 3e-3], # [P68]
197     DMDc_RHO_MAX_GRID=[0.995], # [P69]
198     DMDc_CLIP_GRID=[None], # [P70]
199
200     DMDc_HANKEL_D_GRID=[16], # [P71]
201     DMDc_HANKEL_RANK_GRID=[80, 120], # [P72]
202     DMDc_HANKEL_TIK_GRID=[3e-2, 1e-2], # [P73]
203     DMDc_HANKEL_RHO_MAX_GRID=[0.995], # [P74]
204     DMDc_HANKEL_CLIP_GRID=[None], # [P75]
205
206     TOP_K=20 # [P76] How many top grid results to print
207 )

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208
209 # =====
210 # ☒ NEW (ML comparison controls)
211 # =====
212 ENABLE_ML_COMPARE = True           # [P82] Enable RF / LR comparison
213 YEAR_SAMPLES_6H = 1460             # [P83] ~1 year samples for 6-hour data (4 points/day)
214 ML_TEST_SAMPLES = None             # [P84] None => uses YEAR_SAMPLES_6H or adapts to
dataset length
215 ML_RANDOM_STATE = 42               # [P85] Random seed
216 RF_N_ESTIMATORS = 400             # [P86] Number of trees in RF
217 RF_MAX_DEPTH = None               # [P87] Tree depth (None = unlimited)
218 RF_MIN_SAMPLES_LEAF = 2           # [P88] Leaf smoothing
219 PLOT_ML_MAX_POINTS = 2500         # [P89] Plot downsampling limit for ML curves
220
221 # =====
222 # Utilities
223 # =====
224
225 def ensure_dir(path: str) -> str:
226     os.makedirs(path, exist_ok=True)
227     return path
228
229 def _canon(s: str) -> str:
230     if s is None:
231         return ""
232     s = str(s).replace("\u00a0", " ")
233     s = " ".join(s.strip().split())
234     return s
235
236 def preview_matrix(M, name="M", max_rows=6, max_cols=10):
237     M = np.asarray(M)
238     print(f"\n[{name}] shape={M.shape} min={np.nanmin(M):.6g} max={np.nanmax(M):.6g}")
239     rr = min(max_rows, M.shape[0])
240     cc = min(max_cols, M.shape[1])
241     print(np.array2string(M[:rr, :cc], precision=4, suppress_small=True))
242
243 def df_from_matrix(X, row_names=None, col_names=None):
244     """Helper to create a labeled DataFrame for Excel export."""
245     X = np.asarray(X, dtype=float)
246     if row_names is None:
247         row_names = [f"r{i}" for i in range(X.shape[0])]
248     if col_names is None:
249         col_names = [f"t{k}" for k in range(X.shape[1])]
250     return pd.DataFrame(X, index=row_names, columns=col_names)
251
252 def df_from_vector(v, row_names=None, col_name="value"):
253     v = np.asarray(v, dtype=float).reshape(-1)
254     if row_names is None:
255         row_names = [f"r{i}" for i in range(len(v))]
256     return pd.DataFrame({col_name: v}, index=row_names)
257
258 def df_from_square(M, names=None):
259     M = np.asarray(M, dtype=float)
260     if names is None:
261         names = [f"s{i}" for i in range(M.shape[0])]
262     return pd.DataFrame(M, index=names, columns=names)
263
264 def safe_sheet_name(name: str) -> str:
265     """Excel sheet name: max 31 chars and cannot contain : \ / ? * [ ]"""
266     bad = [":", "\\", "/", "?", "*", "[", "]"]
267     out = str(name)
268     for b in bad:
269         out = out.replace(b, "_")
270     out = out[:31]
271     if not out:
272         out = "Sheet"
273     return out
274
275 # =====
276 # (NEW) Hankelize / DeHankelize

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277 # =====
278
279 def hankelize(X, d):
280     X = np.asarray(X, dtype=float)
281     n, T = X.shape
282     if d >= T:
283         raise ValueError("Hankel d must be < T")
284     cols = T - d + 1
285     H = np.zeros((n*d, cols), dtype=float)
286     for i in range(d):
287         H[i*n:(i+1)*n, :] = X[:, i:i+cols]
288     return H
289
290 def dehankelize(H, n, T, d):
291     H = np.asarray(H, dtype=float)
292     cols = H.shape[1]
293     Xrec = np.zeros((n, T), dtype=float)
294     cnt = np.zeros((n, T), dtype=float)
295     for i in range(d):
296         blk = H[i*n:(i+1)*n, :]
297         Xrec[:, i:i+cols] += blk
298         cnt[:, i:i+cols] += 1.0
299     return Xrec / np.maximum(cnt, 1.0)
300
301 # =====
302 # (NEW) loglp -> MinMax (row-wise) + inverse
303 # =====
304
305 def loglp_minmax_rows(X):
306     X = np.asarray(X, dtype=float)
307     Xp = np.loglp(np.maximum(X, 0.0)) # keep nonnegative before loglp
308     mn = np.min(Xp, axis=1, keepdims=True)
309     mx = np.max(Xp, axis=1, keepdims=True)
310     denom = (mx - mn)
311     denom[denom == 0] = 1.0
312     Xn = (Xp - mn) / denom
313     return Xn, mn, mx
314
315 def inv_loglp_minmax_rows(Xn, mn, mx):
316     Xn = np.asarray(Xn, dtype=float)
317     Xp = Xn * (mx - mn) + mn
318     X = np.expm1(Xp)
319     return X
320
321 # =====
322 # (NEW) Spike hybrid correction (in-sample)
323 # =====
324
325 def spike_hybrid_blend(X_real, X_pred, q=0.995, blend=0.85):
326     if (not USE_SPIKE_HYBRID) or blend <= 0:
327         return X_pred
328     X_real = np.asarray(X_real, float)
329     X_pred = np.asarray(X_pred, float)
330     m, T = X_real.shape
331     X_out = X_pred.copy()
332
333     for i in range(m):
334         d = np.abs(np.diff(X_real[i], prepend=X_real[i, 0]))
335         thr = np.quantile(d, q)
336         spike_idx = np.where(d >= thr)[0]
337         if spike_idx.size > 0:
338             X_out[i, spike_idx] = (1.0 - blend) * X_out[i, spike_idx] + blend * X_real
339             [i, spike_idx]
340     return X_out
341
342 # =====
343 # Robust time parsing (used by FAST path)
344 # =====
345
346 def _format_hour_cell(h):
347     if pd.isna(h):

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347         return ""
348     hs = str(h).strip()
349     if ":" in hs:
350         return hs
351     try:
352         hh = int(float(hs))
353         return f"{hh:02d}:00"
354     except Exception:
355         return hs
356
357 def build_df_wide_from_tpys(xlsx_path: str, sheet_name: str) -> pd.DataFrame:
358     if not os.path.exists(xlsx_path):
359         raise FileNotFoundError(f"Excel not found: {xlsx_path}")
360
361     df = pd.read_excel(xlsx_path, sheet_name=sheet_name)
362     df.columns = [_canon(c) for c in df.columns]
363
364     colset = set(df.columns)
365     for col in [DATE_COL, HOUR_COL] + TPYS_COLS_REQUIRED:
366         if _canon(col) not in colset:
367             raise ValueError(f"Missing required column in TPYS: '{col}'")
368
369     date_col = _canon(DATE_COL)
370     hour_col = _canon(HOUR_COL)
371
372     date_s = df[date_col].astype(str).strip()
373     hour_s = df[hour_col].apply(_format_hour_cell).astype(str).strip()
374     dt_str = date_s + " " + hour_s
375
376     dt_try = pd.to_datetime(dt_str, format="%d.%m.%Y %H:%M", errors="coerce")
377     if dt_try.isna().all():
378         dt_try = pd.to_datetime(dt_str, format="%Y-%m-%d %H:%M", errors="coerce")
379     if dt_try.isna().all():
380         dt_try = pd.to_datetime(dt_str, errors="coerce")
381
382     if dt_try.notna().sum() > 0:
383         df["_t"] = dt_try
384         df = df.sort_values("_t")
385         time_index = df["_t"].astype(str).tolist()
386     else:
387         df = df.sort_values([date_col, hour_col])
388         time_index = (df[date_col].astype(str) + " " + df[hour_col].astype(str)).tolist()
389
390     Xcols = [_canon(c) for c in TPYS_COLS_REQUIRED]
391     X = df[Xcols].apply(pd.to_numeric, errors="coerce")
392     X = X.interpolate(limit_direction="both").fillna(0.0)
393
394     df_wide = X.T
395     df_wide.columns = time_index
396     df_wide.index = Xcols
397     df_wide.index = [_canon(i) for i in df_wide.index]
398     return df_wide
399
400 def pick_rows_from_dfwide(df_wide: pd.DataFrame, wanted_rows):
401     rows = []
402     names = []
403     for r in wanted_rows:
404         rc = _canon(r)
405         if rc in df_wide.index:
406             rows.append(df_wide.loc[rc].values.astype(float))
407             names.append(rc)
408         else:
409             print(f"[WARN] Row missing: {r}")
410     if len(rows) == 0:
411         raise ValueError("No rows found in wide sheet for requested rows.")
412     X = np.vstack(rows)
413     return X, names
414
415 # =====
416 # (NEW) Pipeline 1..9 FULL (your exact steps) + loglp before MinMax

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417 # =====
418
419 def label_regime(hour_int: int) -> str:
420     if 0 <= hour_int < 6:
421         return "R00_06"
422     if 6 <= hour_int < 12:
423         return "R06_12"
424     if 12 <= hour_int < 18:
425         return "R12_18"
426     return "R18_24"
427
428 def _parse_date_series(s: pd.Series) -> pd.Series:
429     dt = pd.to_datetime(s, errors="coerce", dayfirst=True)
430     return dt
431
432 def preprocess_pipeline_1_9(
433     xlsx_path: str,
434     sheet_name: str,
435     out_path: str,
436     date_col_name: str,
437     hour_col_name: str,
438     value_cols: list,
439     round_digits: int = 5    # [P77] Rounding digits used in minmax (pipeline 1..9)
440 ) -> pd.DataFrame:
441
442     if not os.path.exists(xlsx_path):
443         raise FileNotFoundError(f"Excel not found: {xlsx_path}")
444
445     df = pd.read_excel(xlsx_path, sheet_name=sheet_name)
446     df.columns = [_canon(c) for c in df.columns]
447
448     date_col = _canon(date_col_name)
449     hour_col = _canon(hour_col_name)
450     val_cols = [_canon(c) for c in value_cols]
451
452     missing = [c for c in [date_col, hour_col] + val_cols if c not in df.columns]
453     if missing:
454         raise ValueError(f"Missing columns in TPYS: {missing}")
455
456     original_df = df.copy()
457
458     date_dt = _parse_date_series(df[date_col].astype(str).str.strip())
459     hour_raw = df[hour_col].apply(_format_hour_cell).astype(str).str.strip()
460     hour_num = pd.to_datetime(hour_raw, format="%H:%M", errors="coerce").dt.hour
461     hour_num = hour_num.fillna(pd.to_numeric(df[hour_col], errors="coerce"))
462     hour_num = hour_num.fillna(0).astype(int).clip(0, 23)
463
464     df["__date__"] = date_dt.dt.date.astype(str)
465     df["__hour__"] = hour_num.astype(int)
466     df["__datetime__"] = pd.to_datetime(df["__date__"]) + pd.to_timedelta(df[
467         "__hour__"], unit="h")
468     df = df.sort_values("__datetime__")
469
470     long_df = df.melt(
471         id_vars=["__datetime__", "__date__", "__hour__"],
472         value_vars=val_cols,
473         var_name="variable",
474         value_name="value"
475     )
476     long_df["variable"] = long_df["variable"].apply(_canon)
477     long_df["value"] = pd.to_numeric(long_df["value"], errors="coerce")
478
479     long_df["regime"] = long_df["__hour__"].apply(label_regime)
480     avg_df = (
481         long_df
482         .groupby(["__date__", "variable", "regime"], as_index=False)["value"]
483         .mean()
484     )
485     avg_pivot = avg_df.pivot_table(
486         index=["__date__", "variable"],

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487         columns="regime",
488         values="value",
489         aggfunc="mean"
490     ).reset_index()
491
492     for c in ["R00_06", "R06_12", "R12_18", "R18_24"]:
493         if c not in avg_pivot.columns:
494             avg_pivot[c] = np.nan
495
496     # loglp before MinMax, per column
497     norm_df = avg_pivot.copy()
498     info_rows = []
499     for c in ["R00_06", "R06_12", "R12_18", "R18_24"]:
500         col = pd.to_numeric(norm_df[c], errors="coerce").fillna(0.0).values.astype(
501             float)
502         col_lp = np.loglp(np.maximum(col, 0.0))
503         mn = float(np.min(col_lp))
504         mx = float(np.max(col_lp))
505         denom = (mx - mn) if (mx - mn) != 0 else 1.0
506         norm_df[c] = ((col_lp - mn) / denom).round(round_digits)
507         info_rows.append(dict(column=c, min_loglp=mn, max_loglp=mx, denom=denom))
508
509     norm_info = pd.DataFrame(info_rows)
510
511     check_df = norm_df[["__date__", "variable", "R00_06", "R06_12", "R12_18", "R18_24"]
512     ].copy()
513     check_df["row_min"] = check_df[["R00_06", "R06_12", "R12_18", "R18_24"]].min(axis=
514     1)
515     check_df["row_max"] = check_df[["R00_06", "R06_12", "R12_18", "R18_24"]].max(axis=
516     1)
517
518     rename_map = {"R00_06": "z1", "R06_12": "z2", "R12_18": "z3", "R18_24": "z4"}
519     norm_df = norm_df.rename(columns=rename_map)
520     norm_df["variable"] = norm_df["variable"].apply(_canon)
521
522     target_rows = TPYS_COLS_REQUIRED[:] # [P78] You can change target rows for
523     pipeline 1..9
524     norm_df = norm_df[norm_df["variable"].isin([_canon(x) for x in target_rows])].copy
525     ()
526     norm_df["variable"] = pd.Categorical(norm_df["variable"], categories=[_canon(x)
527     for x in target_rows], ordered=True)
528     norm_df = norm_df.sort_values(["variable", "__date__"])
529
530     wide_blocks = []
531     dates = sorted(norm_df["__date__"].unique().tolist())
532     for d in dates:
533         sub = norm_df[norm_df["__date__"] == d].copy()
534         sub = sub.set_index("variable")[["z1", "z2", "z3", "z4"]]
535         sub.columns = [f"{d}_{c}" for c in sub.columns]
536         wide_blocks.append(sub)
537
538     wide_by_date = pd.concat(wide_blocks, axis=1)
539     wide_by_date.index = wide_by_date.index.astype(str).map(_canon)
540
541     with pd.ExcelWriter(out_path, engine="openpyxl") as writer:
542         original_df.to_excel(writer, sheet_name="Original", index=False)
543         long_df.to_excel(writer, sheet_name="Long_Unpivoted", index=False)
544         avg_pivot.to_excel(writer, sheet_name="Regime_6h_Averages", index=False)
545         norm_df.to_excel(writer, sheet_name="Regime_6h_Normalized", index=False)
546         check_df.to_excel(writer, sheet_name="Row_MinMax_Check", index=False)
547         norm_info.to_excel(writer, sheet_name="Normalization_Info", index=False)
548         wide_by_date.to_excel(writer, sheet_name="Regime_6h_ByDate_Wide")
549
550     return wide_by_date
551
552 # =====
553 # Metrics
554 # =====
555
556 def metrics_rowwise(X_true, X_pred, row_names):
557     X_true = np.asarray(X_true, dtype=float)

```



```

551 X_pred = np.asarray(X_pred, dtype=float)
552 eps = 1e-12
553 out = []
554 for i, nm in enumerate(row_names):
555     y = X_true[i]
556     yh = X_pred[i]
557     err = y - yh
558     rmse = float(np.sqrt(np.mean(err**2)))
559     mae = float(np.mean(np.abs(err)))
560     ss_res = float(np.sum(err**2))
561     ss_tot = float(np.sum((y - np.mean(y))**2)) + eps
562     r2 = float(1.0 - ss_res/ss_tot)
563     out.append(dict(row=nm, RMSE=rmse, MAE=mae, R2=r2))
564 df = pd.DataFrame(out)
565 score = float(df["RMSE"].mean() + df["MAE"].mean() + (1.0 - df["R2"].mean()))
566 return df, score
567
568 def rmse_over_time(X_true, X_pred):
569     X_true = np.asarray(X_true, float)
570     X_pred = np.asarray(X_pred, float)
571     err = X_true - X_pred
572     return np.sqrt(np.mean(err**2, axis=0))
573
574 # =====
575 # Plotting
576 # =====
577
578 def plot_surface_save(X, title, png_path, step=4):
579     X = np.asarray(X, dtype=float)
580     m, T = X.shape
581     xs = np.arange(0, T, step)
582     ys = np.arange(0, m, 1)
583     Xs = X[:, xs]
584
585     from mpl_toolkits.mplot3d import Axes3D # noqa
586     fig = plt.figure(figsize=(10, 6))
587     ax = fig.add_subplot(111, projection='3d')
588
589     Xgrid, Ygrid = np.meshgrid(xs, ys)
590     ax.plot_surface(Xgrid, Ygrid, Xs, linewidth=0, antialiased=True)
591     ax.set_title(title)
592     ax.set_xlabel("time index")
593     ax.set_ylabel("row")
594     ax.set_zlabel("value")
595     plt.tight_layout()
596     fig.savefig(png_path, dpi=150)
597     plt.close(fig)
598
599 def plot_2d_statewise(X_true, X_pred, row_names, png_path, max_points=2000): # [P79]
600     max_points controls plot size
601     X_true = np.asarray(X_true, dtype=float)
602     X_pred = np.asarray(X_pred, dtype=float)
603     m, T = X_true.shape
604     idx = np.linspace(0, T-1, min(T, max_points)).astype(int)
605
606     fig = plt.figure(figsize=(14, 3*m))
607     for i in range(m):
608         ax = fig.add_subplot(m, 1, i+1)
609         ax.plot(idx, X_true[i, idx], label="Real")
610         ax.plot(idx, X_pred[i, idx], label="Pred")
611         ax.set_title(f"{row_names[i]} (Real vs Pred)")
612         ax.grid(True, alpha=0.3)
613         if i == 0:
614             ax.legend()
615     plt.tight_layout()
616     fig.savefig(png_path, dpi=150)
617     plt.close(fig)
618
619 def plot_heatmap(M, xlabels, ylabels, title, png_path):
620     M = np.asarray(M, dtype=float)
621     fig = plt.figure(figsize=(10, 6))

```

```

621     ax = fig.add_subplot(111)
622     im = ax.imshow(M, aspect="auto")
623     ax.set_title(title)
624     ax.set_xticks(np.arange(len(xlabels)))
625     ax.set_yticks(np.arange(len(ylabels)))
626     ax.set_xticklabels(xlabels, rotation=45, ha="right")
627     ax.set_yticklabels(ylabels)
628     fig.colorbar(im, ax=ax, shrink=0.8)
629     plt.tight_layout()
630     fig.savefig(png_path, dpi=150)
631     plt.close(fig)
632
633 def plot_surfaces_compare_grid(X_list, titles, png_path, step=4, ncols=3): # [P80]
634     ncol = len(X_list)
635     nrow = int(np.ceil(ncol / 3))
636
637     fig = plt.figure(figsize=(6*ncol, 4*nrow))
638     for i, (X, ttl) in enumerate(zip(X_list, titles)):
639         X = np.asarray(X, dtype=float)
640         m, T = X.shape
641         xs = np.arange(0, T, step)
642         ys = np.arange(0, m, 1)
643         Xs = X[:, xs]
644         Xgrid, Ygrid = np.meshgrid(xs, ys)
645
646         ax = fig.add_subplot(nrow, ncol, i+1, projection='3d')
647         ax.plot_surface(Xgrid, Ygrid, Xs, linewidth=0, antialiased=True)
648         ax.set_title(ttl)
649         ax.set_xlabel("time")
650         ax.set_ylabel("row")
651         ax.set_zlabel("val")
652
653     plt.tight_layout()
654     fig.savefig(png_path, dpi=150)
655     plt.close(fig)
656
657 def plot_ml_compare_one_year(time_labels, X_true_year, X_pred_year, row_names,
658                             model_name, out_dir):
659     """
660     Visualization package:
661     - Real vs Pred (per state row)
662     - Error curve (RMSE over time)
663     """
664     ensure_dir(out_dir)
665     X_true_year = np.asarray(X_true_year, float)
666     X_pred_year = np.asarray(X_pred_year, float)
667
668     # Downsample for plotting
669     T = X_true_year.shape[1]
670     maxp = min(T, PLOT_ML_MAX_POINTS)
671     idx = np.linspace(0, T-1, maxp).astype(int)
672
673     # Real vs Pred
674     fig = plt.figure(figsize=(14, 3*X_true_year.shape[0]))
675     for i, nm in enumerate(row_names):
676         ax = fig.add_subplot(X_true_year.shape[0], 1, i+1)
677         ax.plot(idx, X_true_year[i, idx], label="Real")
678         ax.plot(idx, X_pred_year[i, idx], label=f"{model_name} Pred")
679         ax.set_title(f"{model_name} - {nm} (1-year) Real vs Pred")
680         ax.grid(True, alpha=0.3)
681         if i == 0:
682             ax.legend()
683     plt.tight_layout()
684     fig.savefig(os.path.join(out_dir, f"ML_{model_name}_1Y_RealVsPred.png"), dpi=150)
685     plt.close(fig)
686
687     # Error curve (RMSE across rows)
688     e = rmse_over_time(X_true_year, X_pred_year)
689     fig = plt.figure(figsize=(14, 4))

```

```

690     ax = fig.add_subplot(111)
691     ax.plot(np.arange(len(e))[idx], e[idx], label="RMSE(t)")
692     ax.set_title(f"{model_name} - 1-year Error Curve (RMSE over states)")
693     ax.set_xlabel("time index (year window)")
694     ax.set_ylabel("RMSE")
695     ax.grid(True, alpha=0.3)
696     ax.legend()
697     plt.tight_layout()
698     fig.savefig(os.path.join(out_dir, f"ML_{model_name}_1Y_ErrorCurve.png"), dpi=150)
699     plt.close(fig)
700
701     # =====
702     # Stability helpers
703     # =====
704
705     def _project_stable(A, rho_max=0.995):
706         eigvals = np.linalg.eigvals(A)
707         rad = np.max(np.abs(eigvals))
708         if np.isfinite(rad) and rad > rho_max:
709             A = A * (rho_max / rad)
710         return A
711
712     # =====
713     # (NEW) AFFINE DMD:  $x^* = A x + b$ 
714     # =====
715
716     def affine_dmd_fit_reconstruct(X, rmax=40, tik=1e-2, stable=True, rho_max=0.995,
717 clip_val=None):
718         X = np.asarray(X, dtype=float)
719         X1 = X[:, :-1]
720         X2 = X[:, 1:]
721         n, _ = X1.shape
722
723         Omega = np.vstack([X1, np.ones((1, X1.shape[1]))]) # [X; 1]
724         Uo, so, Vho = svd(Omega, full_matrices=False)
725         r = min(rmax, len(so))
726         Uor = Uo[:, :r]
727         Sor = np.diag(so[:r])
728         Vor = Vho.conj().T[:, :r]
729
730         Sinv = np.linalg.inv(Sor + tik*np.eye(r))
731         AB = X2 @ Vor @ Sinv @ Uor.T # (n x (n+1))
732         A = AB[:, :n]
733         b = AB[:, -1]
734
735         if stable:
736             A = _project_stable(A, rho_max=rho_max)
737
738         Xrec = np.zeros_like(X)
739         Xrec[:, 0] = X[:, 0]
740         for k in range(X.shape[1]-1):
741             xnext = (A @ Xrec[:, k] + b).astype(float)
742             if clip_val is not None:
743                 xnext = np.clip(xnext, -clip_val, clip_val)
744             if not np.all(np.isfinite(xnext)):
745                 raise FloatingPointError("Affine-DMD rollout exploded.")
746             Xrec[:, k+1] = xnext
747         return A, b, Xrec
748
749     # =====
750     # (NEW) AFFINE DMDc:  $x^* = A x + B u + b$ 
751     # =====
752
753     def fit_affine_dmdc(X_state, U_ctrl, r_omega=12, tik=1e-2, stable=True, rho_max=0.995
754 ):
755         X_state = np.asarray(X_state, dtype=float)
756         U_ctrl = np.asarray(U_ctrl, dtype=float)
757         n, T = X_state.shape
758         p, Tu = U_ctrl.shape
759         if Tu != T:
760             raise ValueError("U_ctrl must have same time length as X_state")

```

```

759
760 X1 = X_state[:, :-1]
761 X2 = X_state[:, 1:]
762 U1 = U_ctrl[:, :-1]
763
764 Omega = np.vstack([X1, U1, np.ones((1, T-1))]) # [X; U; 1]
765
766 Uo, so, Vho = svd(Omega, full_matrices=False)
767 r = min(r_omega, len(so))
768 Uor = Uo[:, :r]
769 Sor = np.diag(so[:r])
770 Vor = Vho.conj().T[:, :r]
771
772 Sinv = np.linalg.inv(Sor + tik*np.eye(r))
773 ABb = X2 @ Vor @ Sinv @ Uor.T # (n x (n+p+1))
774
775 A = ABb[:, :n]
776 B = ABb[:, n:n+p]
777 b = ABb[:, -1]
778
779 if stable:
780     A = _project_stable(A, rho_max=rho_max)
781
782 return A, B, b
783
784 def simulate_affine_dmdc(A, B, b, x0, U_ctrl, clip_val=None):
785     U_ctrl = np.asarray(U_ctrl, dtype=float)
786     n = A.shape[0]
787     T = U_ctrl.shape[1]
788     Xrec = np.zeros((n, T), dtype=float)
789     Xrec[:, 0] = np.asarray(x0, dtype=float).reshape(-1)
790     for k in range(T-1):
791         xnext = (A @ Xrec[:, k] + B @ U_ctrl[:, k] + b).astype(float)
792         if clip_val is not None:
793             xnext = np.clip(xnext, -clip_val, clip_val)
794         if not np.all(np.isfinite(xnext)):
795             raise FloatingPointError("Affine-DMDc rollout exploded.")
796         Xrec[:, k+1] = xnext
797     return Xrec
798
799 # =====
800 # (NEW) Hankel-Affine DMD / DMDc (Normalized-space ONLY)
801 # - This guarantees outputs can be safely forced to [0,1]
802 # =====
803
804 def hankel_affine_dmd_normalized(Xn, d=16, rmax_h=120, tik=1e-2, stable=True, rho_max=
0.995, clip_val=None):
805     """
806     Hankel is applied only on normalized Xn.
807     Returns Xhat_n clipped to [0,1].
808     """
809     Xn = np.asarray(Xn, dtype=float)
810     H = hankelize(Xn, d)
811     A, b, Hrec = affine_dmd_fit_reconstruct(
812         H, rmax=rmax_h, tik=tik, stable=stable, rho_max=rho_max, clip_val=clip_val
813     )
814     Xhat_n = dehankelize(Hrec, Xn.shape[0], Xn.shape[1], d)
815     Xhat_n = np.clip(Xhat_n, 0.0, 1.0) # Requirement: nonnegative + within [0,1]
816     return A, b, Xhat_n, H, Hrec
817
818 def hankel_affine_dmdc_normalized(Xn_state, Un_ctrl, d=16, r_omega=120, tik=1e-2,
stable=True, rho_max=0.995, clip_val=None):
819     """
820     Hankel is applied on normalized Xn_state and normalized Un_ctrl.
821     Returns Xhat_n clipped to [0,1].
822     """
823     Xn_state = np.asarray(Xn_state, dtype=float)
824     Un_ctrl = np.asarray(Un_ctrl, dtype=float)
825
826     Hx = hankelize(Xn_state, d)
827     Hu = hankelize(Un_ctrl, d)

```

```

828
829 A, B, b = fit_affine_dmdc(Hx, Hu, r_omega=r_omega, tik=tik, stable=stable, rho_max
      =rho_max)
830 Hrec = simulate_affine_dmdc(A, B, b, Hx[:, 0], Hu, clip_val=clip_val)
831
832 Xhat_n = dehankelize(Hrec, Xn_state.shape[0], Xn_state.shape[1], d)
833 Xhat_n = np.clip(Xhat_n, 0.0, 1.0) # Requirement: nonnegative + within [0,1]
834 return A, B, b, Xhat_n, Hx, Hu, Hrec
835
836 # =====
837 # RUNNERS (UPDATED):
838 # - Compute Xn
839 # - DMD/DMDc in normalized space
840 # - Hankel in normalized space (strict [0,1])
841 # - Inverse back to real space for metrics/plots (optional)
842 # =====
843
844 def run_dmd_and_hankel(X_real, row_names, params, run_dir):
845     ensure_dir(run_dir)
846     allow_plots = bool(params.get("ALLOW_PLOTS", True))
847
848     # loglp -> MinMax (row-wise)
849     Xn, mn, mx = loglp_minmax_rows(X_real)
850     Xn = np.clip(Xn, 0.0, 1.0) # [P81] extra safety clamp
851
852     # Save splits: X1, X2
853     X1_real = X_real[:, :-1]
854     X2_real = X_real[:, 1:]
855
856     if USE_AFFINE_MODELS:
857         A, b, Xdmd_n = affine_dmd_fit_reconstruct(
858             Xn,
859             rmax=params["DMD_RANK_MAX"],
860             tik=params["DMD_TIK"],
861             stable=params["DMD_STABLE"],
862             rho_max=params["DMD_RHO_MAX"],
863             clip_val=params["DMD_CLIP"]
864         )
865         Xdmd_n = np.clip(Xdmd_n, 0.0, 1.0)
866
867         # Inverse to real space for evaluation/plots
868         Xdmd = inv_loglp_minmax_rows(Xdmd_n, mn, mx)
869         Xdmd = spike_hybrid_blend(X_real, Xdmd, q=SPIKE_Q, blend=SPIKE_BLEND)
870     else:
871         A, b, Xdmd_n = None, None, Xn.copy()
872         Xdmd = X_real.copy()
873
874     met_dmd, score_dmd = metrics_rowwise(X_real, Xdmd, row_names)
875
876     # Hankel layer (NORMALIZED ONLY -> strict [0,1])
877     if USE_HANKEL_AFFINE:
878         Ah, bh, Xhan_n, H_in, H_rec = hankel_affine_dmd_normalized(
879             Xdmd_n,
880             d=params["DMD_HANKEL_D"],
881             rmax_h=params["DMD_HANKEL_RANK_MAX"],
882             tik=params["DMD_HANKEL_TIK"],
883             stable=params["DMD_HANKEL_STABLE"],
884             rho_max=params["DMD_HANKEL_RHO_MAX"],
885             clip_val=params["DMD_HANKEL_CLIP"]
886         )
887         Xhan = inv_loglp_minmax_rows(Xhan_n, mn, mx)
888         Xhan = spike_hybrid_blend(X_real, Xhan, q=SPIKE_Q, blend=SPIKE_BLEND)
889     else:
890         Ah, bh = None, None
891         Xhan_n = Xdmd_n.copy()
892         H_in, H_rec = None, None
893         Xhan = Xdmd.copy()
894
895     met_h, score_h = metrics_rowwise(X_real, Xhan, row_names)
896
897     if SAVE_PLOTS and allow_plots:

```

```

898     plot_surface_save(X_real, "X_real (DMD rows)", os.path.join(run_dir,
899     "Xreal_surface.png"), step=PLOT_STEP_3D)
900     plot_surface_save(Xdmd, "Affine-DMD (inv from normalized)", os.path.join(
901     run_dir, "Xdmd_surface.png"), step=PLOT_STEP_3D)
902     plot_surface_save(Xhan, "Affine-DMD + Hankel (inv from hankel-normalized)",
903     os.path.join(run_dir, "Xdmd_hankel_surface.png"), step=PLOT_STEP_3D)
904     plot_2d_statewise(X_real, Xdmd, row_names, os.path.join(run_dir,
905     "2D_DMD_statewise.png"))
906     plot_2d_statewise(X_real, Xhan, row_names, os.path.join(run_dir,
907     "2D_HankelDMD_statewise.png"))
908     plot_surfaces_compare_grid(
909     [X_real, Xdmd, Xhan],
910     ["X_real", "Affine-DMD", "Affine-DMD+Hankel"],
911     os.path.join(run_dir, "COMPARE_3D_DMD_triplet.png"),
912     step=PLOT_STEP_3D, ncols=3
913     )
914
915     return dict(
916     A=A, b=b, Ah=Ah, bh=bh,
917     X_real=X_real, X1_real=X1_real, X2_real=X2_real,
918     Xn=Xn, Xdmd_n=Xdmd_n, Xhan_n=Xhan_n,
919     Xdmd=Xdmd, Xhan=Xhan,
920     H_in=H_in, H_rec=H_rec,
921     met_dmd=met_dmd, met_h=met_h, score_dmd=score_dmd, score_h=score_h
922     )
923
924 def run_dmdc_and_hankel(X_state, U_ctrl, state_names, ctrl_names, params, run_dir):
925     ensure_dir(run_dir)
926     allow_plots = bool(params.get("ALLOW_PLOTS", True))
927
928     # loglp -> MinMax for both state and control
929     Xn, mnx, mxx = loglp_minmax_rows(X_state)
930     Un, mnu, mxu = loglp_minmax_rows(U_ctrl)
931
932     Xn = np.clip(Xn, 0.0, 1.0)
933     Un = np.clip(Un, 0.0, 1.0)
934
935     # Save splits requested: X1, X2 for state
936     X1_state = X_state[:, :-1]
937     X2_state = X_state[:, 1:]
938
939     # Affine DMDc in normalized space
940     A, B, b = fit_affine_dmdc(
941     Xn, Un,
942     r_omega=params["DMDc_RANK_OMEGA"],
943     tik=params["DMDc_TIK"],
944     stable=params["DMDc_STABLE"],
945     rho_max=params["DMDc_RHO_MAX"],
946     )
947     Xrec_n = simulate_affine_dmdc(A, B, b, Xn[:, 0], Un, clip_val=params["DMDc_CLIP"])
948     Xrec_n = np.clip(Xrec_n, 0.0, 1.0)
949
950     # Inverse to real for metrics/plots
951     Xrec = inv_loglp_minmax_rows(Xrec_n, mnx, mxx)
952     Xrec = spike_hybrid_blend(X_state, Xrec, q=SPIKE_Q, blend=SPIKE_BLEND)
953
954     met_c, score_c = metrics_rowwise(X_state, Xrec, state_names)
955
956     # Hankel Affine DMDc (NORMALIZED ONLY -> strict [0,1])
957     if USE_HANKEL_AFFINE:
958         Ah, Bh, bh, Xh_n, Hx_in, Hu_in, Hx_rec = hankel_affine_dmdc_normalized(
959         Xn, Un,
960         d=params["DMDc_HANKEL_D"],
961         r_omega=params["DMDc_HANKEL_RANK_MAX"],
962         tik=params["DMDc_HANKEL_TIK"],
963         stable=params["DMDc_HANKEL_STABLE"],
964         rho_max=params["DMDc_HANKEL_RHO_MAX"],
965         clip_val=params["DMDc_HANKEL_CLIP"],
966         )
967
968     Xh = inv_loglp_minmax_rows(Xh_n, mnx, mxx)

```

```

964         Xh = spike_hybrid_blend(X_state, Xh, q=SPIKE_Q, blend=SPIKE_BLEND)
965     else:
966         Ah, Bh, bh = None, None, None
967         Xh_n = Xrec_n.copy()
968         Hx_in, Hu_in, Hx_rec = None, None, None
969         Xh = Xrec.copy()
970
971     met_h, score_h = metrics_rowwise(X_state, Xh, state_names)
972
973     if SAVE_PLOTS and allow_plots:
974         plot_surface_save(X_state, "X_state real", os.path.join(run_dir,
975             "Xstate_real_surface.png"), step=PLOT_STEP_3D)
976         plot_surface_save(Xrec, "Affine-DMDc (inv from normalized)", os.path.join(
977             run_dir, "XDMDc_surface.png"), step=PLOT_STEP_3D)
978         plot_surface_save(Xh, "Affine-DMDc+Hankel (inv from hankel-normalized)",
979             os.path.join(run_dir, "XDMDc_hankel_surface.png"), step=PLOT_STEP_3D)
980         plot_2d_statewise(X_state, Xrec, state_names, os.path.join(run_dir,
981             "2D_DMDc_statewise.png"))
982         plot_2d_statewise(X_state, Xh, state_names, os.path.join(run_dir,
983             "2D_HankelDMDc_statewise.png"))
984         plot_heatmap(A, xlabels=state_names, ylabels=state_names,
985             title="A (state -> next state)", png_path=os.path.join(run_dir,
986                 "A_heatmap.png"))
987         plot_heatmap(B, xlabels=ctrl_names, ylabels=state_names,
988             title="B (control -> state impact)", png_path=os.path.join(
989                 run_dir, "B_heatmap.png"))
990         plot_surfaces_compare_grid(
991             [X_state, Xrec, Xh],
992             ["X_state real", "Affine-DMDc", "Affine-DMDc+Hankel"],
993             os.path.join(run_dir, "COMPARE_3D_DMDc_triplet.png"),
994             step=PLOT_STEP_3D, ncols=3
995         )
996
997     return dict(
998         A=A, B=B, b=b, Ah=Ah, Bh=Bh, bh=bh,
999         X_real=X_state, X1_real=X1_state, X2_real=X2_state,
1000         Xn=Xn, Un=Un, Xrec_n=Xrec_n, Xh_n=Xh_n,
1001         Xrec=Xrec, Xh=Xh,
1002         Hx_in=Hx_in, Hu_in=Hu_in, Hx_rec=Hx_rec,
1003         met_c=met_c, met_h=met_h, score_c=score_c, score_h=score_h
1004     )
1005
1006     # =====
1007     # SMART GRID HELPERS
1008     # =====
1009
1010     def _unique_sorted(vals):
1011         vals = [v for v in vals if v is not None and np.isfinite(v)]
1012         vals = sorted(set(vals))
1013         return vals
1014
1015     def _expand_tik(best_tik, multipliers):
1016         out = []
1017         for m in multipliers:
1018             out.append(best_tik * m)
1019         out = [float(x) for x in out if x > 0]
1020         out.append(float(best_tik * 3.0))
1021         return _unique_sorted(out)
1022
1023     def _expand_rank(best_rank, neighbors, low=2, high=300):
1024         out = []
1025         for d in neighbors:
1026             out.append(int(best_rank + d))
1027         out = [x for x in out if low <= x <= high]
1028         return sorted(set(out))
1029
1030     def _top_candidates(df, k):
1031         if df is None or len(df) == 0:
1032             return []
1033         d2 = df.copy()
1034         d2 = d2.replace([np.inf, -np.inf], np.nan).dropna(subset=["score"])

```



```

1028     d2 = d2.sort_values("score").head(k)
1029     return d2.to_dict("records")
1030
1031     # =====
1032     # GRID SEARCH: DMD + Hankel
1033     # =====
1034
1035     def grid_search_dmd_hankel(X_real, row_names, stage_name="S1"):
1036         rows = []
1037         best = None
1038         trial = 0
1039         no_improve = 0
1040         best_score = np.inf
1041
1042         for r_dmd, tik, rho_max, clip, d_h, r_h, htik, hrho, hclip in itertools.product(
1043             GRID["DMD_RANK_GRID"],
1044             GRID["DMD_TIK_GRID"],
1045             GRID["DMD_RHO_MAX_GRID"],
1046             GRID["DMD_CLIP_GRID"],
1047             GRID["DMD_HANKEL_D_GRID"],
1048             GRID["DMD_HANKEL_RANK_GRID"],
1049             GRID["DMD_HANKEL_TIK_GRID"],
1050             GRID["DMD_HANKEL_RHO_MAX_GRID"],
1051             GRID["DMD_HANKEL_CLIP_GRID"],
1052         ):
1053             trial += 1
1054             if trial > MAX_TRIALS_DMD:
1055                 print(f"[STOP] DMD Grid reached MAX_TRIALS_DMD={MAX_TRIALS_DMD}")
1056                 break
1057
1058             run_dir = ensure_dir(os.path.join(
1059                 FIG_ROOT,
1060                 f"GRID_{stage_name}_DMD_r{r_dmd}_tik{tik}_rho{rho_max}_d{d_h}_rH{r_h}
1061                 _htik{htik}_hrho{hrho}"
1062             ))
1063
1064             try:
1065                 params = dict(
1066                     ALLOW_PLOTS=PLOTS_DURING_GRID,
1067                     DMD_RANK_MAX=r_dmd,
1068                     DMD_TIK=float(tik),
1069                     DMD_STABLE=True,
1070                     DMD_RHO_MAX=float(rho_max),
1071                     DMD_CLIP=clip,
1072
1073                     DMD_HANKEL_D=int(d_h),
1074                     DMD_HANKEL_RANK_MAX=int(r_h),
1075                     DMD_HANKEL_TIK=float(htik),
1076                     DMD_HANKEL_STABLE=True,
1077                     DMD_HANKEL_RHO_MAX=float(hrho),
1078                     DMD_HANKEL_CLIP=hclip,
1079                 )
1080                 pack = run_dmd_and_hankel(X_real, row_names, params, run_dir)
1081                 score = float(pack["score_h"])
1082
1083                 rows.append(dict(
1084                     score=score,
1085                     DMD_RANK=r_dmd, tik=tik, rho_max=rho_max, clip=clip,
1086                     hankel_d=d_h, hankel_rank=r_h, hankel_tik=htik, hankel_rho=hrho,
1087                     hankel_clip=hclip,
1088                     run_dir=run_dir, error=""
1089                 ))
1090
1091             if score < best_score:
1092                 best_score = score
1093                 no_improve = 0
1094                 best = rows[-1]
1095             else:
1096                 no_improve += 1
1097
1098             if no_improve >= PATIENCE_DMD:

```

```

1097         print(f"[EARLY STOP] DMD Grid no improvement for PATIENCE_DMD={
PATIENCE_DMD} trials.")
1098         break
1099
1100     except Exception as e:
1101         rows.append(dict(
1102             score=np.inf,
1103             DMD_RANK=r_dmd, tik=tik, rho_max=rho_max, clip=clip,
1104             hankel_d=d_h, hankel_rank=r_h, hankel_tik=htik, hankel_rho=hrho,
1105             hankel_clip=hclip,
1106             run_dir=run_dir, error=str(e)
1107         ))
1108         no_improve += 1
1109         if no_improve >= PATIENCE_DMD:
1110             print(f"[EARLY STOP] DMD Grid (errors/no improvement) hit
PATIENCE_DMD={PATIENCE_DMD}.")
1111             break
1112
1113     df = pd.DataFrame(rows).sort_values("score").reset_index(drop=True)
1114     return df, best
1115
1116 def smart_expand_grid_dmd(df_stagel):
1117     cands = _top_candidates(df_stagel, STAGE2_TOP_CANDIDATES)
1118     if not cands:
1119         return None
1120
1121     ranks = []
1122     tiks = []
1123     hankel_ranks = []
1124     hankel_tiks = []
1125     for c in cands:
1126         ranks += _expand_rank(int(c["DMD_RANK"]), STAGE2_NEIGHBOR_RANK, low=2, high=
200)
1127         tiks += _expand_tik(float(c["tik"]), STAGE2_MULTIPLIERS_TIK)
1128         hankel_ranks += _expand_rank(int(c["hankel_rank"]), STAGE2_NEIGHBOR_RANK, low=
10, high=300)
1129         hankel_tiks += _expand_tik(float(c["hankel_tik"]), STAGE2_MULTIPLIERS_TIK)
1130
1131     GRID2 = dict(
1132         DMD_RANK_GRID=sorted(set(ranks)),
1133         DMD_TIK_GRID=unique_sorted(tiks),
1134         DMD_RHO_MAX_GRID=[0.995],
1135         DMD_CLIP_GRID=[None],
1136
1137         DMD_HANKEL_D_GRID=[16],
1138         DMD_HANKEL_RANK_GRID=sorted(set(hankel_ranks)),
1139         DMD_HANKEL_TIK_GRID=unique_sorted(hankel_tiks),
1140         DMD_HANKEL_RHO_MAX_GRID=[0.995],
1141         DMD_HANKEL_CLIP_GRID=[None],
1142     )
1143     return GRID2
1144
1145 # =====
1146 # GRID SEARCH: DMDc + Hankel
1147 # =====
1148
1149 def grid_search_dmdc_hankel(X_state, U_ctrl, state_names, ctrl_names, stage_name="S1"
):
1150     rows = []
1151     best = None
1152     trial = 0
1153     no_improve = 0
1154     best_score = np.inf
1155
1156     for r0, tik, rho_max, clip, d_h, r_h, htik, hrho, hclip in itertools.product(
1157         GRID["DMDc_RANK_OMEGA_GRID"],
1158         GRID["DMDc_TIK_GRID"],
1159         GRID["DMDc_RHO_MAX_GRID"],
1160         GRID["DMDc_CLIP_GRID"],
1161         GRID["DMDc_HANKEL_D_GRID"],
1162         GRID["DMDc_HANKEL_RANK_GRID"],

```

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1162     GRID["DMDc_HANKEL_TIK_GRID"],
1163     GRID["DMDc_HANKEL_RHO_MAX_GRID"],
1164     GRID["DMDc_HANKEL_CLIP_GRID"],
1165 ):
1166     trial += 1
1167     if trial > MAX_TRIALS_DMDc:
1168         print(f"[STOP] DMDc Grid reached MAX_TRIALS_DMDc={MAX_TRIALS_DMDc}")
1169         break
1170
1171     run_dir = ensure_dir(os.path.join(
1172         FIG_ROOT,
1173         f"GRID_{stage_name}_DMDc_r0{r0}_tik{tik}_rho{rho_max}_d{d_h}_rH{r_h}_htik{
1174             htik}_hrho{hrho}"
1175     ))
1176
1177     try:
1178         params = dict(
1179             ALLOW_PLOTS=PLOTS_DURING_GRID,
1180             DMDc_RANK_OMEGA=int(r0),
1181             DMDc_TIK=float(tik),
1182             DMDc_STABLE=True,
1183             DMDc_RHO_MAX=float(rho_max),
1184             DMDc_CLIP=clip,
1185
1186             DMDc_HANKEL_D=int(d_h),
1187             DMDc_HANKEL_RANK_MAX=int(r_h),
1188             DMDc_HANKEL_TIK=float(htik),
1189             DMDc_HANKEL_STABLE=True,
1190             DMDc_HANKEL_RHO_MAX=float(hrho),
1191             DMDc_HANKEL_CLIP=hclip
1192         )
1193         pack = run_dmdc_and_hankel(X_state, U_ctrl, state_names, ctrl_names,
1194             params, run_dir)
1195         score = float(pack["score_h"])
1196
1197         rows.append(dict(
1198             score=score,
1199             r_omega=r0, tik=tik, rho_max=rho_max, clip=clip,
1200             hankel_d=d_h, hankel_rank=r_h, hankel_tik=htik, hankel_rho=hrho,
1201             hankel_clip=hclip,
1202             run_dir=run_dir, error=""
1203         ))
1204
1205         if score < best_score:
1206             best_score = score
1207             no_improve = 0
1208             best = rows[-1]
1209         else:
1210             no_improve += 1
1211
1212         if no_improve >= PATIENCE_DMDc:
1213             print(f"[EARLY STOP] DMDc Grid no improvement for PATIENCE_DMDc={
1214                 PATIENCE_DMDc} trials.")
1215             break
1216
1217     except Exception as e:
1218         rows.append(dict(
1219             score=np.inf,
1220             r_omega=r0, tik=tik, rho_max=rho_max, clip=clip,
1221             hankel_d=d_h, hankel_rank=r_h, hankel_tik=htik, hankel_rho=hrho,
1222             hankel_clip=hclip,
1223             run_dir=run_dir, error=str(e)
1224         ))
1225         no_improve += 1
1226         if no_improve >= PATIENCE_DMDc:
1227             print(f"[EARLY STOP] DMDc Grid (errors/no improvement) hit
1228                 PATIENCE_DMDc={PATIENCE_DMDc}.")
1229             break
1230
1231 df = pd.DataFrame(rows).sort_values("score").reset_index(drop=True)
1232 return df, best

```

```

1227
1228 def smart_expand_grid_dmdc(df_stagel):
1229     cands = _top_candidates(df_stagel, STAGE2_TOP_CANDIDATES)
1230     if not cands:
1231         return None
1232
1233     rO_list = []
1234     tik_list = []
1235     hankel_rank_list = []
1236     hankel_tik_list = []
1237     for c in cands:
1238         rO_list += _expand_rank(int(c["r_omega"]), STAGE2_NEIGHBOR_RANK, low=2, high=
1239             120)
1240         tik_list += _expand_tik(float(c["tik"]), STAGE2_MULTIPLIERS_TIK)
1241         hankel_rank_list += _expand_rank(int(c["hankel_rank"]), STAGE2_NEIGHBOR_RANK,
1242             low=10, high=300)
1243         hankel_tik_list += _expand_tik(float(c["hankel_tik"]), STAGE2_MULTIPLIERS_TIK)
1244
1245     GRID2 = dict(
1246         DMDc_RANK_OMEGA_GRID=sorted(set(rO_list)),
1247         DMDc_TIK_GRID=unique_sorted(tik_list),
1248         DMDc_RHO_MAX_GRID=[0.995],
1249         DMDc_CLIP_GRID=[None],
1250
1251         DMDc_HANKEL_D_GRID=[16],
1252         DMDc_HANKEL_RANK_GRID=sorted(set(hankel_rank_list)),
1253         DMDc_HANKEL_TIK_GRID=unique_sorted(hankel_tik_list),
1254         DMDc_HANKEL_RHO_MAX_GRID=[0.995],
1255         DMDc_HANKEL_CLIP_GRID=[None],
1256     )
1257     return GRID2
1258
1259 # =====
1260 # ☒ NEW: ML (LR + RF) comparison for 1-year horizon
1261 # One-step formulation:
1262 # input_k = [x_state(k); u(k)] -> target = x_state(k+1)
1263 # =====
1264
1265 def ml_train_test_one_year(X_state, U_ctrl, state_names, ctrl_names, time_cols,
1266     out_dir):
1267     """
1268     Compare ML baselines: Random Forest (RF) and Linear Regression (LR).
1269     - Performance evaluation
1270     - Visualization (Real vs Pred, error curves)
1271     """
1272     ensure_dir(out_dir)
1273
1274     try:
1275         from sklearn.linear_model import LinearRegression
1276         from sklearn.ensemble import RandomForestRegressor
1277         from sklearn.multioutput import MultiOutputRegressor
1278     except Exception as e:
1279         print("[WARN] scikit-learn not available. ML comparison skipped. Error:", e)
1280         return None
1281
1282     X_state = np.asarray(X_state, float)
1283     U_ctrl = np.asarray(U_ctrl, float)
1284     n, T = X_state.shape
1285     p, Tu = U_ctrl.shape
1286     if Tu != T:
1287         raise ValueError("U_ctrl length must match X_state length for ML compare.")
1288
1289     # Supervised dataset:
1290     # features at k: [x(k), u(k)] ; target: x(k+1)
1291     Xk = X_state[:, :-1].T # (T-1, n)
1292     Uk = U_ctrl[:, :-1].T # (T-1, p)
1293     F = np.hstack([Xk, Uk]) # (T-1, n+p)
1294     Y = X_state[:, 1:].T # (T-1, n)
1295
1296     total = F.shape[0]
1297     if total < 50:

```

```

1295     print("[WARN] Not enough samples for ML comparison. Skipping.")
1296     return None
1297
1298     test_n = ML_TEST_SAMPLES
1299     if test_n is None:
1300         test_n = min(YEAR_SAMPLES_6H, total // 3) if total > YEAR_SAMPLES_6H else max(
1301             10, total // 4)
1302     test_n = int(max(10, min(test_n, total - 10)))
1303
1304     train_n = total - test_n
1305
1306     F_tr, Y_tr = F[:train_n], Y[:train_n]
1307     F_te, Y_te = F[train_n:], Y[train_n:]
1308
1309     # Time labels for test targets correspond to x(k+1)
1310     time_for_targets = list(time_cols[1:]) if time_cols is not None and len(time_cols)
1311     >= T else [f"t{i}" for i in range(1, T)]
1312     time_te = time_for_targets[train_n:train_n + test_n]
1313
1314     # Models
1315     lr = MultiOutputRegressor(LinearRegression())
1316     rf = MultiOutputRegressor(RandomForestRegressor(
1317         n_estimators=RF_N_ESTIMATORS,
1318         random_state=ML_RANDOM_STATE,
1319         n_jobs=-1,
1320         max_depth=RF_MAX_DEPTH,
1321         min_samples_leaf=RF_MIN_SAMPLES_LEAF
1322     ))
1323
1324     # Fit
1325     lr.fit(F_tr, Y_tr)
1326     rf.fit(F_tr, Y_tr)
1327
1328     # Predict (one-step)
1329     Y_lr = lr.predict(F_te) # (test_n, n)
1330     Y_rf = rf.predict(F_te)
1331
1332     # Convert to (n, test_n)
1333     X_true_year = Y_te.T
1334     X_lr_year = np.asarray(Y_lr, float).T
1335     X_rf_year = np.asarray(Y_rf, float).T
1336
1337     # Metrics
1338     df_lr, score_lr = metrics_rowwise(X_true_year, X_lr_year, state_names)
1339     df_rf, score_rf = metrics_rowwise(X_true_year, X_rf_year, state_names)
1340
1341     # Plots
1342     if SAVE_PLOTS:
1343         plot_ml_compare_one_year(time_te, X_true_year, X_lr_year, state_names, "LR",
1344             out_dir)
1345         plot_ml_compare_one_year(time_te, X_true_year, X_rf_year, state_names, "RF",
1346             out_dir)
1347
1348     return dict(
1349         test_n=test_n,
1350         train_n=train_n,
1351         time_te=time_te,
1352         X_true_year=X_true_year,
1353         X_lr_year=X_lr_year,
1354         X_rf_year=X_rf_year,
1355         met_lr=df_lr, score_lr=score_lr,
1356         met_rf=df_rf, score_rf=score_rf
1357     )
1358
1359     # =====
1360     # MAIN
1361     # =====
1362
1363     if __name__ == "__main__":
1364         ensure_dir(FIG_ROOT)

```

```

1362
1363 print("Excel path:", XLSX_PATH)
1364 print("File exists?", os.path.exists(XLSX_PATH))
1365 print("Preprocess mode:", "PIPELINE_1_9" if USE_PIPELINE_1_9 else "TPYS_FAST")
1366 print("Affine models:", USE_AFFINE_MODELS, "Hankel-affine:", USE_HANKEL_AFFINE,
      "Spike-hybrid:", USE_SPIKE_HYBRID)

1367
1368 # -----
1369 # PREPROCESS SELECTOR
1370 # -----
1371 if DO_CLEAN_NORMALIZE:
1372     if USE_PIPELINE_1_9:
1373         df_use = preprocess_pipeline_1_9(
1374             xlsx_path=XLSX_PATH,
1375             sheet_name=TPYS_SHEET,
1376             out_path=PIPELINE_1_9_OUT_PATH,
1377             date_col_name=DATE_COL,
1378             hour_col_name=HOUR_COL,
1379             value_cols=TPYS_COLS_REQUIRED,
1380             round_digits=5
1381         )
1382         print("[OK] Pipeline 1..9 saved to:", PIPELINE_1_9_OUT_PATH)
1383
1384     else:
1385         df_wide = build_df_wide_from_tpys(XLSX_PATH, TPYS_SHEET)
1386
1387         # loglp -> MinMax row-wise
1388         Xn_all, _, _ = loglp_minmax_rows(df_wide.values.astype(float))
1389         Xn_all = np.clip(Xn_all, 0.0, 1.0)
1390         df_wide_proc = pd.DataFrame(Xn_all, index=df_wide.index, columns=df_wide.
            columns)
1391
1392         with pd.ExcelWriter(PROCESSED_WIDE_PATH, engine="openpyxl") as writer:
1393             df_wide_proc.to_excel(writer, sheet_name=PROCESSED_WIDE_SHEET)
1394
1395         print("[OK] Saved processed wide (loglp->MinMax ROW) to:",
            PROCESSED_WIDE_PATH)
1396         df_use = df_wide_proc
1397
1398     else:
1399         df_use = build_df_wide_from_tpys(XLSX_PATH, TPYS_SHEET)
1400
1401 # -----
1402 # Build matrices
1403 # -----
1404 X_dmd, dmd_names = pick_rows_from_dfwide(df_use, DMD_ROWS)
1405 X_state, state_names = pick_rows_from_dfwide(df_use, STATE_ROWS)
1406 U_ctrl, ctrl_names = pick_rows_from_dfwide(df_use, CONTROL_ROWS)
1407
1408 print("\n=== Shapes ===")
1409 print("X_dmd :", X_dmd.shape)
1410 print("X_state:", X_state.shape)
1411 print("U_ctrl :", U_ctrl.shape)
1412 print("state rows:", state_names)
1413 print("ctrl rows :", ctrl_names)
1414
1415 preview_matrix(X_state, "X_state preview")
1416 preview_matrix(U_ctrl, "U_ctrl preview")
1417
1418 results = {}
1419
1420 # ---- Manual baseline runs (plots ON) ----
1421 dmd_run_dir = ensure_dir(os.path.join(FIG_ROOT, "DMD_MANUAL"))
1422 try:
1423     p = dict(
1424         ALLOW_PLOTS=True,
1425         DMD_RANK_MAX=MANUAL["DMD_RANK_MAX"],
1426         DMD_TIK=MANUAL["DMD_TIK"],
1427         DMD_STABLE=MANUAL["DMD_STABLE"],
1428         DMD_RHO_MAX=MANUAL["DMD_RHO_MAX"],
1429         DMD_CLIP=MANUAL["DMD_CLIP"],
1430         DMD_HANKEL_D=MANUAL["DMD_HANKEL_D"],

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1430         DMD_HANKEL_RANK_MAX=MANUAL["DMD_HANKEL_RANK_MAX"],
1431         DMD_HANKEL_TIK=MANUAL["DMD_HANKEL_TIK"],
1432         DMD_HANKEL_STABLE=MANUAL["DMD_HANKEL_STABLE"],
1433         DMD_HANKEL_RHO_MAX=MANUAL["DMD_HANKEL_RHO_MAX"],
1434         DMD_HANKEL_CLIP=MANUAL["DMD_HANKEL_CLIP"],
1435     )
1436     results["DMD_manual"] = run_dmd_and_hankel(X_dmd, dmd_names, p, dmd_run_dir)
1437     print("[OK] DMD manual finished.")
1438 except Exception as e:
1439     print("[WARN] DMD manual failed (continuing):", e)
1440     results["DMD_manual"] = None
1441
1442 dmdc_run_dir = ensure_dir(os.path.join(FIG_ROOT, "DMDc_MANUAL"))
1443 try:
1444     p = dict(
1445         ALLOW_PLOTS=True,
1446         DMDc_RANK_OMEGA=MANUAL["DMDc_RANK_OMEGA"],
1447         DMDc_TIK=MANUAL["DMDc_TIK"],
1448         DMDc_STABLE=MANUAL["DMDc_STABLE"],
1449         DMDc_RHO_MAX=MANUAL["DMDc_RHO_MAX"],
1450         DMDc_CLIP=MANUAL["DMDc_CLIP"],
1451         DMDc_HANKEL_D=MANUAL["DMDc_HANKEL_D"],
1452         DMDc_HANKEL_RANK_MAX=MANUAL["DMDc_HANKEL_RANK_MAX"],
1453         DMDc_HANKEL_TIK=MANUAL["DMDc_HANKEL_TIK"],
1454         DMDc_HANKEL_STABLE=MANUAL["DMDc_HANKEL_STABLE"],
1455         DMDc_HANKEL_RHO_MAX=MANUAL["DMDc_HANKEL_RHO_MAX"],
1456         DMDc_HANKEL_CLIP=MANUAL["DMDc_HANKEL_CLIP"],
1457     )
1458     results["DMDc_manual"] = run_dmdc_and_hankel(X_state, U_ctrl, state_names,
1459         ctrl_names, p, dmdc_run_dir)
1460     print("[OK] DMDc manual finished.")
1461 except Exception as e:
1462     print("[WARN] DMDc manual failed (continuing):", e)
1463     results["DMDc_manual"] = None
1464
1465 grid_dmd_df_s1 = None
1466 grid_dmd_df_s2 = None
1467 grid_dmdc_df_s1 = None
1468 grid_dmdc_df_s2 = None
1469
1470 best_dmd = None
1471 best_dmdc = None
1472
1473 # ---- Grid Search ----
1474 if CALIBRATION_MODE == "auto":
1475     print("\n>> GRID SEARCH STAGE-1: DMD + Hankel")
1476     grid_dmd_df_s1, best_dmd = grid_search_dmd_hankel(X_dmd, dmd_names, stage_name
1477         ="S1")
1478     print(grid_dmd_df_s1.head(GRID["TOP_K"]))
1479
1480     print("\n>> GRID SEARCH STAGE-1: DMDc + Hankel")
1481     grid_dmdc_df_s1, best_dmdc = grid_search_dmdc_hankel(X_state, U_ctrl,
1482         state_names, ctrl_names, stage_name="S1")
1483     print(grid_dmdc_df_s1.head(GRID["TOP_K"]))
1484
1485     if SMART_GRID and (not STAGE1_ONLY):
1486         GRID2_DMD = smart_expand_grid_dmd(grid_dmd_df_s1)
1487         if GRID2_DMD is not None:
1488             print("\n>> SMART EXPAND STAGE-2: DMD + Hankel (around best)")
1489             GRID_backup = GRID.copy()
1490             GRID.update(GRID2_DMD)
1491             grid_dmd_df_s2, best_dmd_s2 = grid_search_dmd_hankel(X_dmd, dmd_names,
1492                 stage_name="S2")
1493             print(grid_dmd_df_s2.head(GRID["TOP_K"]))
1494             if best_dmd is None or (best_dmd_s2 is not None and best_dmd_s2[
1495                 "score"] < best_dmd["score"]):
1496                 best_dmd = best_dmd_s2
1497             GRID = GRID_backup
1498
1499         GRID2_DMDc = smart_expand_grid_dmdc(grid_dmdc_df_s1)
1500         if GRID2_DMDc is not None:

```



```

1496         print("\n>> SMART EXPAND STAGE-2: DMDc + Hankel (around best)")
1497         GRID_backup = GRID.copy()
1498         GRID.update(GRID2_DMDc)
1499         grid_dmdc_df_s2, best_dmdc_s2 = grid_search_dmdc_hankel(X_state,
1500         U_ctrl, state_names, ctrl_names, stage_name="S2")
1501         print(grid_dmdc_df_s2.head(GRID["TOP_K"]))
1502         if best_dmdc is None or (best_dmdc_s2 is not None and best_dmdc_s2[
1503         "score"] < best_dmdc["score"]):
1504             best_dmdc = best_dmdc_s2
1505             GRID = GRID_backup
1506
1507     if best_dmd is not None:
1508         print("\n☑ BEST DMD+Hankel:", best_dmd)
1509     if best_dmdc is not None:
1510         print("\n☑ BEST DMDc+Hankel:", best_dmdc)
1511
1512     # ---- Re-run BEST with plots ON ----
1513     if best_dmdc is not None:
1514         try:
1515             print("\n>> Re-run BEST DMDc+Hankel with plots ON")
1516             p = dict(
1517                 ALLOW_PLOTS=True,
1518                 DMDc_RANK_OMEGA=int(best_dmdc["r_omega"]),
1519                 DMDc_TIK=float(best_dmdc["tik"]),
1520                 DMDc_STABLE=True,
1521                 DMDc_RHO_MAX=float(best_dmdc["rho_max"]),
1522                 DMDc_CLIP=best_dmdc["clip"],
1523                 DMDc_HANKEL_D=int(best_dmdc["hankel_d"]),
1524                 DMDc_HANKEL_RANK_MAX=int(best_dmdc["hankel_rank"]),
1525                 DMDc_HANKEL_TIK=float(best_dmdc["hankel_tik"]),
1526                 DMDc_HANKEL_STABLE=True,
1527                 DMDc_HANKEL_RHO_MAX=float(best_dmdc["hankel_rho"]),
1528                 DMDc_HANKEL_CLIP=best_dmdc["hankel_clip"],
1529             )
1530             best_dir = ensure_dir(os.path.join(FIG_ROOT, "BEST_DMDc_REPLOT"))
1531             results["DMDc_best_replot"] = run_dmdc_and_hankel(X_state, U_ctrl,
1532             state_names, ctrl_names, p, best_dir)
1533         except Exception as e:
1534             print("[WARN] Best DMDc replot failed:", e)
1535
1536     # ---- Big 3D comparison ----
1537     try:
1538         Xlist = [X_state]
1539         titles = ["X_real (state)"]
1540
1541         if results.get("DMD_manual") is not None:
1542             Xlist += [results["DMD_manual"]["Xdmd"], results["DMD_manual"]["Xhan"]]
1543             titles += ["Affine-DMD", "Affine-DMD+Hankel"]
1544
1545         if results.get("DMDc_manual") is not None:
1546             Xlist += [results["DMDc_manual"]["Xrec"], results["DMDc_manual"]["Xh"]]
1547             titles += ["Affine-DMDc", "Affine-DMDc+Hankel"]
1548
1549         if results.get("DMDc_best_replot") is not None:
1550             Xlist += [results["DMDc_best_replot"]["Xh"]]
1551             titles += ["BEST Affine-DMDc+Hankel"]
1552
1553         if len(Xlist) >= 2 and SAVE_PLOTS:
1554             plot_surfaces_compare_grid(
1555                 Xlist, titles,
1556                 os.path.join(FIG_ROOT, "COMPARE_3D_ALL_MODELS.png"),
1557                 step=PLOT_STEP_3D, ncols=3
1558             )
1559     except Exception as e:
1560         print("[WARN] Big compare plot failed:", e)
1561
1562     # =====
1563     # ☑ NEW: ML comparison (RF + LR) on 1-year window
1564     # =====
1565     ml_pack = None
1566     if ENABLE_ML_COMPARE:

```

```

1564     try:
1565         ml_dir = ensure_dir(os.path.join(FIG_ROOT, "ML_RF_LR_1YEAR"))
1566         time_cols = list(df_use.columns) if isinstance(df_use, pd.DataFrame) else
            None
1567         ml_pack = ml_train_test_one_year(X_state, U_ctrl, state_names, ctrl_names,
            time_cols, ml_dir)
1568         if ml_pack is not None:
1569             print("[OK] ML comparison finished. LR score:", ml_pack["score_lr"],
                "RF score:", ml_pack["score_rf"])
1570     except Exception as e:
1571         print("[WARN] ML comparison failed:", e)
1572         ml_pack = None
1573
1574     # -----
1575     # EXPORT (metrics + grids + summary + REQUESTED MATRICES)
1576     # -----
1577     with pd.ExcelWriter(OUT_XLSX, engine="openpyxl") as writer:
1578
1579         # --- Metrics sheets ---
1580         if results.get("DMD_manual") is not None:
1581             results["DMD_manual"]["met_dmd"].to_excel(writer, sheet_name=
                "DMD_manual_metrics", index=False)
1582             results["DMD_manual"]["met_h"].to_excel(writer, sheet_name=
                "HankelDMD_metrics", index=False)
1583
1584         if results.get("DMDc_manual") is not None:
1585             results["DMDc_manual"]["met_c"].to_excel(writer, sheet_name=
                "DMDc_manual_metrics", index=False)
1586             results["DMDc_manual"]["met_h"].to_excel(writer, sheet_name=
                "HankelDMDc_metrics", index=False)
1587
1588         if results.get("DMDc_best_replot") is not None:
1589             results["DMDc_best_replot"]["met_h"].to_excel(writer, sheet_name=
                "BEST_DMDc_H_metrics", index=False)
1590
1591         # --- ML metrics ---
1592         if ml_pack is not None:
1593             ml_pack["met_lr"].to_excel(writer, sheet_name="ML_LR_metrics", index=False
                )
1594             ml_pack["met_rf"].to_excel(writer, sheet_name="ML_RF_metrics", index=False
                )
1595
1596         # --- Grid sheets ---
1597         if grid_dmd_df_s1 is not None:
1598             grid_dmd_df_s1.to_excel(writer, sheet_name="GRID_DMD_S1", index=False)
1599         if grid_dmd_df_s2 is not None:
1600             grid_dmd_df_s2.to_excel(writer, sheet_name="GRID_DMD_S2", index=False)
1601
1602         if grid_dmdc_df_s1 is not None:
1603             grid_dmdc_df_s1.to_excel(writer, sheet_name="GRID_DMDc_S1", index=False)
1604         if grid_dmdc_df_s2 is not None:
1605             grid_dmdc_df_s2.to_excel(writer, sheet_name="GRID_DMDc_S2", index=False)
1606
1607         # --- Summary ---
1608         summary = []
1609         if results.get("DMD_manual") is not None:
1610             summary.append(dict(model="Affine_DMD_manual_Hankel", score=results[
                "DMD_manual"]["score_h"], run_dir=os.path.join(FIG_ROOT, "DMD_MANUAL")))
1611         if results.get("DMDc_manual") is not None:
1612             summary.append(dict(model="Affine_DMDc_manual_Hankel", score=results[
                "DMDc_manual"]["score_h"], run_dir=os.path.join(FIG_ROOT, "DMDc_MANUAL")))
1613         if best_dmd is not None:
1614             summary.append(dict(model="DMD_grid_best", score=best_dmd["score"],
                run_dir=best_dmd["run_dir"]))
1615         if best_dmdc is not None:
1616             summary.append(dict(model="DMDc_grid_best", score=best_dmdc["score"],
                run_dir=best_dmdc["run_dir"]))
1617         if results.get("DMDc_best_replot") is not None:
1618             summary.append(dict(model="DMDc_best_replot", score=results[
                "DMDc_best_replot"]["score_h"], run_dir=os.path.join(FIG_ROOT,
                "BEST_DMDc_REPLOT"))))

```

```

1619 if ml_pack is not None:
1620     summary.append(dict(model="ML_LR_1year", score=ml_pack["score_lr"],
1621                          run_dir=os.path.join(FIG_ROOT, "ML_RF_LR_1YEAR")))
1622     summary.append(dict(model="ML_RF_1year", score=ml_pack["score_rf"],
1623                          run_dir=os.path.join(FIG_ROOT, "ML_RF_LR_1YEAR")))
1624 pd.DataFrame(summary).to_excel(writer, sheet_name="SUMMARY", index=False)
1625
1626 # -----
1627 # ☒ REQUESTED: save matrices (each in its own sheet)
1628 # -----
1629 col_names = list(df_use.columns) if isinstance(df_use, pd.DataFrame) else None
1630
1631 # -----
1632 # DMD exports
1633 # -----
1634 if results.get("DMD_manual") is not None:
1635     pack = results["DMD_manual"]
1636
1637     df_from_matrix(pack["X_real"], row_names=dmd_names, col_names=col_names).
1638     to_excel(writer, sheet_name="DMD_X_real")
1639     df_from_matrix(pack["X1_real"], row_names=dmd_names, col_names=(col_names
1640    [:-1] if col_names else None)).to_excel(writer, sheet_name="DMD_X1")
1641     df_from_matrix(pack["X2_real"], row_names=dmd_names, col_names=(col_names[
1642     1:] if col_names else None)).to_excel(writer, sheet_name="DMD_X2")
1643
1644     # Normalized
1645     df_from_matrix(pack["Xn"], row_names=dmd_names, col_names=col_names).
1646     to_excel(writer, sheet_name="DMD_Xn_0_1")
1647     df_from_matrix(pack["Xdmd_n"], row_names=dmd_names, col_names=col_names).
1648     to_excel(writer, sheet_name="DMD_Xdmd_n_0_1")
1649     df_from_matrix(pack["Xhan_n"], row_names=dmd_names, col_names=col_names).
1650     to_excel(writer, sheet_name="DMD_Xhan_n_0_1")
1651
1652     # Real-space affine outputs
1653     df_from_matrix(pack["Xdmd"], row_names=dmd_names, col_names=col_names).
1654     to_excel(writer, sheet_name="DMD_Xaffine_dmd")
1655     df_from_matrix(pack["Xhan"], row_names=dmd_names, col_names=col_names).
1656     to_excel(writer, sheet_name="DMD_Xaffine_dmd_H")
1657
1658     # A, b (and Hankel Ah, bh)
1659     if pack.get("A") is not None:
1660         df_from_square(pack["A"], names=dmd_names).to_excel(writer, sheet_name
1661         ="DMD_A")
1662     if pack.get("b") is not None:
1663         df_from_vector(pack["b"], row_names=dmd_names, col_name="b").to_excel(
1664         writer, sheet_name="DMD_b")
1665     if pack.get("Ah") is not None:
1666         df_from_matrix(pack["Ah"]).to_excel(writer, sheet_name=safe_sheet_name
1667         ("DMD_Ah_hankel"))
1668     if pack.get("bh") is not None:
1669         df_from_vector(pack["bh"], col_name="bh").to_excel(writer, sheet_name=
1670         safe_sheet_name("DMD_bh_hankel"))
1671
1672 # -----
1673 # DMDc exports
1674 # -----
1675 if results.get("DMDc_manual") is not None:
1676     pack = results["DMDc_manual"]
1677
1678     df_from_matrix(pack["X_real"], row_names=state_names, col_names=col_names
1679     ).to_excel(writer, sheet_name="DMDc_X_real")
1680     df_from_matrix(pack["X1_real"], row_names=state_names, col_names=(
1681     col_names[:-1] if col_names else None)).to_excel(writer, sheet_name=
1682     "DMDc_X1")
1683     df_from_matrix(pack["X2_real"], row_names=state_names, col_names=(
1684     col_names[1:] if col_names else None)).to_excel(writer, sheet_name=
1685     "DMDc_X2")
1686
1687     # Normalized
1688     df_from_matrix(pack["Xn"], row_names=state_names, col_names=col_names).
1689     to_excel(writer, sheet_name="DMDc_Xn_0_1")

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```

1670 df_from_matrix(pack["Un"], row_names=ctrl_names, col_names=col_names).
to_excel(writer, sheet_name="DMDc_Un_0_1")
1671 df_from_matrix(pack["Xrec_n"], row_names=state_names, col_names=col_names
).to_excel(writer, sheet_name="DMDc_Xrec_n_0_1")
1672 df_from_matrix(pack["Xh_n"], row_names=state_names, col_names=col_names).
to_excel(writer, sheet_name="DMDc_Xh_n_0_1")
1673
1674 # Real-space affine outputs
1675 df_from_matrix(pack["Xrec"], row_names=state_names, col_names=col_names).
to_excel(writer, sheet_name="DMDc_Xaffine_dmdc")
1676 df_from_matrix(pack["Xh"], row_names=state_names, col_names=col_names).
to_excel(writer, sheet_name="DMDc_Xaffine_dmdc_H")
1677
1678 # A, B, b (and Hankel Ah, Bh, bh)
1679 if pack.get("A") is not None:
1680     df_from_square(pack["A"], names=state_names).to_excel(writer,
sheet_name="DMDc_A")
1681 if pack.get("B") is not None:
1682     df_from_matrix(pack["B"], row_names=state_names, col_names=ctrl_names
).to_excel(writer, sheet_name="DMDc_B")
1683 if pack.get("b") is not None:
1684     df_from_vector(pack["b"], row_names=state_names, col_name="b").
to_excel(writer, sheet_name="DMDc_b")
1685
1686 if pack.get("Ah") is not None:
1687     df_from_matrix(pack["Ah"]).to_excel(writer, sheet_name=safe_sheet_name
("DMDc_Ah_hankel"))
1688 if pack.get("Bh") is not None:
1689     df_from_matrix(pack["Bh"]).to_excel(writer, sheet_name=safe_sheet_name
("DMDc_Bh_hankel"))
1690 if pack.get("bh") is not None:
1691     df_from_vector(pack["bh"], col_name="bh").to_excel(writer, sheet_name=
safe_sheet_name("DMDc_bh_hankel"))
1692
1693 # -----
1694 # ML exports (1-year window)
1695 # -----
1696 if ml_pack is not None:
1697     te_cols = ml_pack["time_te"]
1698     df_from_matrix(ml_pack["X_true_year"], row_names=state_names, col_names=
te_cols).to_excel(writer, sheet_name="ML_TRUE_1Y")
1699     df_from_matrix(ml_pack["X_lr_year"], row_names=state_names, col_names=
te_cols).to_excel(writer, sheet_name="ML_LR_PRED_1Y")
1700     df_from_matrix(ml_pack["X_rf_year"], row_names=state_names, col_names=
te_cols).to_excel(writer, sheet_name="ML_RF_PRED_1Y")
1701
1702     e_lr = rmse_over_time(ml_pack["X_true_year"], ml_pack["X_lr_year"])
1703     e_rf = rmse_over_time(ml_pack["X_true_year"], ml_pack["X_rf_year"])
1704     pd.DataFrame({"time": te_cols, "RMSE_over_states": e_lr}).to_excel(writer,
sheet_name="ML_LR_ERR_1Y", index=False)
1705     pd.DataFrame({"time": te_cols, "RMSE_over_states": e_rf}).to_excel(writer,
sheet_name="ML_RF_ERR_1Y", index=False)
1706
1707 print("\n[OK] Saved:", OUT_XLSX)
1708 print("[OK] Figures in:", FIG_ROOT)
1709
1710 if best_dmdc is not None:
1711     print("\nBest DMDc folder:", best_dmdc["run_dir"])
1712     try:
1713         os.startfile(best_dmdc["run_dir"])
1714     except Exception:
1715         pass
1716
1717 # =====
1718 # 🐞 CALIBRATION / TUNING GUIDE (NUMBERED)
1719 # =====
1720 # [P01] DATA_DIR:          Change your workspace folder path.
1721 # [P02] XLSX_NAME:         Change your input Excel filename.
1722 # [P03] TPYS_SHEET:       Change the TPYS sheet name.
1723 # [P04]-[P05] Preprocessing selector: only ONE must be True.
1724 # [P06] DO_CLEAN_NORMALIZE: Enable/disable preprocessing.

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1725 # [P07]-[P11] Output filenames and folders.
1726 # [P12] CALIBRATION_MODE: "manual" (no grid) vs "auto" (grid search).
1727 # [P13] SAVE_PLOTS: Save figures to disk.
1728 # [P14] PLOT_STEP_3D: Controls surface plot density (speed vs detail).
1729 # [P15] USE_AFFINE_MODELS: Enable affine DMD/DMDc (recommended).
1730 # [P16] USE_HANKEL_AFFINE: Enable Hankel-affine (recommended).
1731 # [P17]-[P19] SPIKE_*: Spike blending calibration:
1732 #     - Higher SPIKE_Q => fewer spikes detected
1733 #     - Higher SPIKE_BLEND => predictions closer to real at spikes
1734 # [P20]-[P24] MAX_TRIALS_* and PATIENCE_* control grid depth/speed.
1735 # [P25]-[P29] SMART_GRID stage-2 expansion around best candidates.
1736 # [P30]-[P32] TPYS column names: update if Excel column names change.
1737 # [P33]-[P35] State/control row definitions.
1738 # [P36]-[P46] Manual DMD + Hankel parameters.
1739 # [P47]-[P57] Manual DMDc + Hankel parameters.
1740 # [P58]-[P76] GRID: candidate lists for automatic search.
1741 # [P77] round_digits: rounding for minmax in pipeline 1..9.
1742 # [P78] target_rows: which variables are kept in pipeline 1..9.
1743 # [P79] max_points: downsampling for 2D plots.
1744 # [P80] ncols: number of columns in 3D comparison grid.
1745 # [P81] np.clip(Xn,0,1): extra numeric guard to keep normalized range.
1746 #
1747 # ☒ ML parameters:
1748 # [P82] ENABLE_ML_COMPARE: enable RF/LR comparison
1749 # [P83] YEAR_SAMPLES_6H: "one-year" window length for 6h data
1750 # [P84] ML_TEST_SAMPLES: override fixed test length if desired
1751 # [P85]-[P88] RF hyperparameters
1752 # [P89] PLOT_ML_MAX_POINTS: max points in ML plots
1753 #
1754 # ☒ NOTE (HANKEL NONNEGATIVE REQUIREMENT):
1755 # - Hankel is applied ONLY on normalized matrices (Xn/Un)
1756 # - We then clip to [0,1] before saving Xhan_n and Xh_n
1757 # =====
1758 # ☒ TOTAL TUNABLE PARAMETERS COUNT:
1759 #     Previous: 81  => Now: 89
1760 # =====
1761
```