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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 + (log1p -> 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 kodlarim"    # [P01] Workspace folder path
# (change if your files moved)
50 XLSX_NAME = "DGP_0-1_Kodlu_Talimat_Hacimleri_regime6h_NORMALIZED.xlsx"    # [P02] Input
# Excel filename
51 XLSX_PATH = os.path.join(DATA_DIR, XLSX_NAME)
52
53 TPYS_SHEET = "TPYS"    # [P03] Sheet name containing TPYS data
54
55 # -----
56 # (NEW) Choose ONE preprocessing mode
57 # -----
58 USE_PIPELINE_1_9 = True        # [P04] True => Pipeline 1..9 FULL
59 USE_TPYS_FAST = False        # [P05] True => TPYS FAST + log1p->MinMax row-wise
60
61 if USE_PIPELINE_1_9 == USE_TPYS_FAST:
62     raise ValueError("Choose exactly ONE preprocessing mode: set
# USE_PIPELINE_1_9=True and USE_TPYS_FAST=False (or vice versa).")
63
64 DO_CLEAN_NORMALIZE = True      # [P06] True => run preprocessing (clean/normalize).
# False => only read wide
65
66 # Output for pipeline 1..9 workbook
67 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
142 experiments)
143
144 # -----
145 # 3) MANUAL PARAMS (baseline)
146 # -----
147 MANUAL = dict(
148     # ---- DMD ----
149     DMD_RANK_MAX=40,           # [P36]
150     DMD_TIK=1e-2,             # [P37]
151     DMD_STABLE=True,          # [P38]
152     DMD_RHO_MAX=0.995,        # [P39]
153     DMD_CLIP=None,            # [P40] Clip for rollout (None disables)
154
155     # Hankel-DMD
156     DMD_HANKEL_D=16,          # [P41] Hankel window length d
157     DMD_HANKEL_RANK_MAX=120,   # [P42]
158     DMD_HANKEL_TIK=1e-2,       # [P43]
159     DMD_HANKEL_STABLE=True,    # [P44]
160     DMD_HANKEL_RHO_MAX=0.995, # [P45]
161     DMD_HANKEL_CLIP=None,      # [P46]
162
163     # ---- DMDC ----
164     DMDC_RANK_OMEGA=12,       # [P47]
165     DMDC_TIK=1e-2,             # [P48]
166     DMDC_STABLE=True,          # [P49]
167     DMDC_RHO_MAX=0.995,        # [P50]
168     DMDC_CLIP=None,            # [P51]
169
170     # Hankel(DMDC)
171     DMDC_HANKEL_D=16,          # [P52]
172     DMDC_HANKEL_RANK_MAX=120,   # [P53]
173     DMDC_HANKEL_TIK=1e-2,       # [P54]
174     DMDC_HANKEL_STABLE=True,    # [P55]
175     DMDC_HANKEL_RHO_MAX=0.995, # [P56]
176     DMDC_HANKEL_CLIP=None,      # [P57]
177 )
178
179 # -----
180 # 4) GRID SEARCH (Stage-1 safe)
181 # -----
182 GRID = dict(
183     # --- DMD + Hankel Stage-1 ---
184     DMD_RANK_GRID=[20, 40],      # [P58]
185     DMD_TIK_GRID=[1e-2],          # [P59]
186     DMD_RHO_MAX_GRID=[0.995],    # [P60]
187     DMD_CLIP_GRID=[None],         # [P61]
188
189     DMD_HANKEL_D_GRID=[16],       # [P62]
190     DMD_HANKEL_RANK_GRID=[80, 120], # [P63]
191     DMD_HANKEL_TIK_GRID=[3e-2, 1e-2], # [P64]
192     DMD_HANKEL_RHO_MAX_GRID=[0.995], # [P65]
193     DMD_HANKEL_CLIP_GRID=[None],    # [P66]
194
195     # --- DMDC + Hankel Stage-1 ---
196     DMDC_RANK_OMEGA_GRID=[10, 15], # [P67]
197     DMDC_TIK_GRID=[1e-2, 3e-3],    # [P68]
198     DMDC_RHO_MAX_GRID=[0.995],    # [P69]
199     DMDC_CLIP_GRID=[None],         # [P70]
200
201     DMDC_HANKEL_D_GRID=[16],       # [P71]
202     DMDC_HANKEL_RANK_GRID=[80, 120], # [P72]
203     DMDC_HANKEL_TIK_GRID=[3e-2, 1e-2], # [P73]
204     DMDC_HANKEL_RHO_MAX_GRID=[0.995], # [P74]
205     DMDC_HANKEL_CLIP_GRID=[None],    # [P75]
206
207     TOP_K=20 # [P76] How many top grid results to print
)

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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
215 dataset length
216 ML_RANDOM_STATE = 42            # [P85] Random seed
217 RF_N_ESTIMATORS = 400           # [P86] Number of trees in RF
218 RF_MAX_DEPTH = None             # [P87] Tree depth (None = unlimited)
219 RF_MIN_SAMPLES_LEAF = 2         # [P88] Leaf smoothing
220 PLOT_ML_MAX_POINTS = 2500       # [P89] Plot downsampling limit for ML curves
221
222 # =====
223 # Utilities
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) log1p -> MinMax (row-wise) + inverse
303 # =====
304
305 def log1p_minmax_rows(X):
306     X = np.asarray(X, dtype=float)
307     Xp = np.log1p(np.maximum(X, 0.0)) # keep nonnegative before log1p
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_log1p_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 def _format_hour_cell(h):
346     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_tpyss(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).str.strip()
373     hour_s = df[hour_col].apply(_format_hour_cell).astype(str).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) + log1p 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
486     avg_pivot = avg_df.pivot_table(
487         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     # log1p 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.log1p(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_log1p=mn, max_log1p=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, xlabel, ylabel, 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     ncols controls grid width
635     from mpl_toolkits.mplot3d import Axes3D # noqa
636     n = len(X_list)
637     nrows = int(np.ceil(n / ncols))
638
639     fig = plt.figure(figsize=(6*ncols, 4*nrows))
640     for i, (X, ttl) in enumerate(zip(X_list, titles)):
641         X = np.asarray(X, dtype=float)
642         m, T = X.shape
643         xs = np.arange(0, T, step)
644         ys = np.arange(0, m, 1)
645         Xs = X[:, xs]
646         Xgrid, Ygrid = np.meshgrid(xs, ys)
647
648         ax = fig.add_subplot(nrows, ncols, i+1, projection='3d')
649         ax.plot_surface(Xgrid, Ygrid, Xs, linewidth=0, antialiased=True)
650         ax.set_title(ttl)
651         ax.set_xlabel("time")
652         ax.set_ylabel("row")
653         ax.set_zlabel("val")
654
655     plt.tight_layout()
656     fig.savefig(png_path, dpi=150)
657     plt.close(fig)
658
659 def plot_ml_compare_one_year(time_labels, X_true_year, X_pred_year, row_names,
660                               model_name, out_dir):
661     """
662     Visualization package:
663     - Real vs Pred (per state row)
664     - Error curve (RMSE over time)
665     """
666
667     ensure_dir(out_dir)
668     X_true_year = np.asarray(X_true_year, float)
669     X_pred_year = np.asarray(X_pred_year, float)
670
671     # Downsample for plotting
672     T = X_true_year.shape[1]
673     maxp = min(T, PLOT_ML_MAX_POINTS)
674     idx = np.linspace(0, T-1, maxp).astype(int)
675
676     # Real vs Pred
677     fig = plt.figure(figsize=(14, 3*X_true_year.shape[0]))
678     for i, nm in enumerate(row_names):
679         ax = fig.add_subplot(X_true_year.shape[0], 1, i+1)
680         ax.plot(idx, X_true_year[i, idx], label="Real")
681         ax.plot(idx, X_pred_year[i, idx], label=f"{model_name} Pred")
682         ax.set_title(f"{model_name} - {nm} (1-year) Real vs Pred")
683         ax.grid(True, alpha=0.3)
684         if i == 0:
685             ax.legend()
686     plt.tight_layout()
687     fig.savefig(os.path.join(out_dir, f"ML_{model_name}_1Y_RealVsPred.png"), dpi=150)
688     plt.close(fig)
689
690     # Error curve (RMSE across rows)
691     e = rmse_over_time(X_true_year, X_pred_year)
692     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
748     return A, b, Xrec
749
750 # =====
751 # (NEW) AFFINE DMDc:  $x^* = A x + B u + b$ 
752 # =====
753
754 def fit_affine_dmdc(X_state, U_ctrl, r_omega=12, tik=1e-2, stable=True, rho_max=0.995
755 ):
756     X_state = np.asarray(X_state, dtype=float)
757     U_ctrl = np.asarray(U_ctrl, dtype=float)
758     n, T = X_state.shape
759     p, Tu = U_ctrl.shape
760     if Tu != T:
761         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
830     =rho_max)
831     Hrec = simulate_affine_dmdc(A, B, b, Hx[:, 0], Hu, clip_val=clip_val)
832
833     Xhat_n = dehankelize(Hrec, Xn_state.shape[0], Xn_state.shape[1], d)
834     Xhat_n = np.clip(Xhat_n, 0.0, 1.0) # Requirement: nonnegative + within [0,1]
835
836     return A, B, b, Xhat_n, Hx, Hu, Hrec
837
838 # =====
839 # RUNNERS (UPDATED):
840 #   - Compute Xn
841 #   - DMD/DMDc in normalized space
842 #   - Hankel in normalized space (strict [0,1])
843 #   - Inverse back to real space for metrics/plots (optional)
844 # =====
845
846 def run_dmd_and_hankel(X_real, row_names, params, run_dir):
847     ensure_dir(run_dir)
848     allow_plots = bool(params.get("ALLOW_PLOTS", True))
849
850     # log1p -> MinMax (row-wise)
851     Xn, mn, mx = log1p_minmax_rows(X_real)
852     Xn = np.clip(Xn, 0.0, 1.0) # [P81] extra safety clamp
853
854     # Save splits: X1, X2
855     X1_real = X_real[:, :-1]
856     X2_real = X_real[:, 1:]
857
858     if USE_AFFINE_MODELS:
859         A, b, Xdmd_n = affine_dmd_fit_reconstruct(
860             Xn,
861             rmax=params["DMD_RANK_MAX"],
862             tik=params["DMD_TIK"],
863             stable=params["DMD_STABLE"],
864             rho_max=params["DMD_RHO_MAX"],
865             clip_val=params["DMD_CLIP"])
866
867         Xdmd_n = np.clip(Xdmd_n, 0.0, 1.0)
868
869         # Inverse to real space for evaluation/plots
870         Xdmd = inv_log1p_minmax_rows(Xdmd_n, mn, mx)
871         Xdmd = spike_hybrid_blend(X_real, Xdmd, q=SPIKE_Q, blend=SPIKE_BLEND)
872     else:
873         A, b, Xdmd_n = None, None, Xn.copy()
874         Xdmd = X_real.copy()
875
876         met_dmd, score_dmd = metrics_rowwise(X_real, Xdmd, row_names)
877
878         # Hankel layer (NORMALIZED ONLY -> strict [0,1])
879         if USE_HANKEL_AFFINE:
880             Ah, bh, Xhan_n, H_in, H_rec = hankel_affine_dmd_normalized(
881                 Xdmd_n,
882                 d=params["DMD_HANKEL_D"],
883                 rmax_h=params["DMD_HANKEL_RANK_MAX"],
884                 tik=params["DMD_HANKEL_TIK"],
885                 stable=params["DMD_HANKEL_STABLE"],
886                 rho_max=params["DMD_HANKEL_RHO_MAX"],
887                 clip_val=params["DMD_HANKEL_CLIP"])
888
889             Xhan = inv_log1p_minmax_rows(Xhan_n, mn, mx)
890             Xhan = spike_hybrid_blend(X_real, Xhan, q=SPIKE_Q, blend=SPIKE_BLEND)
891
892         else:
893             Ah, bh = None, None
894             Xhan_n = Xdmd_n.copy()
895             H_in, H_rec = None, None
896             Xhan = Xdmd.copy()
897
898         met_h, score_h = metrics_rowwise(X_real, Xhan, row_names)
899
900         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     # log1p -> MinMax for both state and control
929     Xn, mnx, mxx = log1p_minmax_rows(X_state)
930     Un, mnu, mxu = log1p_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_log1p_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_log1p_minmax_rows(Xh_n, mnx, mxx)

```

```

964     Xh = spike_hybrid_blend(X_state, Xh, q=SPIKE_Q, blend=SPIKE_BLEND)
965
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, xlabel=state_names, ylabel=state_names,
985             title="A (state -> next state)", png_path=os.path.join(run_dir,
986             "A_heatmap.png"))
987         plot_heatmap(B, xlabel=ctrl_names, ylabel=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     )
998
999 # =====
1000 # SMART GRID HELPERS
1001 # =====
1002
1003 def _unique_sorted(vals):
1004     vals = [v for v in vals if v is not None and np.isfinite(v)]
1005     vals = sorted(set(vals))
1006     return vals
1007
1008 def _expand_tik(best_tik, multipliers):
1009     out = []
1010     for m in multipliers:
1011         out.append(best_tik * m)
1012     out = [float(x) for x in out if x > 0]
1013     out.append(float(best_tik * 3.0))
1014     return _unique_sorted(out)
1015
1016 def _expand_rank(best_rank, neighbors, low=2, high=300):
1017     out = []
1018     for d in neighbors:
1019         out.append(int(best_rank + d))
1020     out = [x for x in out if low <= x <= high]
1021     return sorted(set(out))
1022
1023 def _top_candidates(df, k):
1024     if df is None or len(df) == 0:
1025         return []
1026     d2 = df.copy()
1027     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}_htik{htik}_hrho{hrho}""
1061         ))
1062
1063     try:
1064         params = dict(
1065             ALLOW_PLOTS=PLOTS_DURING_GRID,
1066             DMD_RANK_MAX=r_dmd,
1067             DMD_TIK=float(tik),
1068             DMD_STABLE=True,
1069             DMD_RHO_MAX=float(rho_max),
1070             DMD_CLIP=clip,
1071
1072             DMD_HANKEL_D=int(d_h),
1073             DMD_HANKEL_RANK_MAX=int(r_h),
1074             DMD_HANKEL_TIK=float(htik),
1075             DMD_HANKEL_STABLE=True,
1076             DMD_HANKEL_RHO_MAX=float(hrho),
1077             DMD_HANKEL_CLIP=hclip,
1078         )
1079         pack = run_dmd_and_hankel(X_real, row_names, params, run_dir)
1080         score = float(pack["score_h"])
1081
1082         rows.append(dict(
1083             score=score,
1084             DMD_RANK=r_dmd, tik=tik, rho_max=rho_max, clip=clip,
1085             hankel_d=d_h, hankel_rank=r_h, hankel_tik=htik, hankel_rho=hrho,
1086             hankel_clip=hclip,
1087             run_dir=run_dir, error=""
1088         ))
1089
1090         if score < best_score:
1091             best_score = score
1092             no_improve = 0
1093             best = rows[-1]
1094         else:
1095             no_improve += 1
1096
1097         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_stage1):
1117     cands = _top_candidates(df_stage1, 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_rO{rO}_tik{tik}_rho{rho_max}_d{d_h}_rH{r_h}_htik{
1174         htik}_hrho{hrho}" ))
1175
1176   try:
1177     params = dict(
1178       ALLOW_PLOTS=PLOTS_DURING_GRID,
1179       DMDC_RANK_OMEGA=int(rO),
1180       DMDC_TIK=float(tik),
1181       DMDC_STABLE=True,
1182       DMDC_RHO_MAX=float(rho_max),
1183       DMDC_CLIP=clip,
1184
1185       DMDC_HANKEL_D=int(d_h),
1186       DMDC_HANKEL_RANK_MAX=int(r_h),
1187       DMDC_HANKEL_TIK=float(htik),
1188       DMDC_HANKEL_STABLE=True,
1189       DMDC_HANKEL_RHO_MAX=float(hrho),
1190       DMDC_HANKEL_CLIP=hclip
1191     )
1192     pack = run_dmdc_and_hankel(X_state, U_ctrl, state_names, ctrl_names,
1193                               params, run_dir)
1194     score = float(pack["score_h"])
1195
1196     rows.append(dict(
1197       score=score,
1198       r_omega=rO, tik=tik, rho_max=rho_max, clip=clip,
1199       hankel_d=d_h, hankel_rank=r_h, hankel_tik=htik, hankel_rho=hrho,
1200       hankel_clip=hclip,
1201       run_dir=run_dir, error=""
1202     ))
1203
1204     if score < best_score:
1205       best_score = score
1206       no_improve = 0
1207       best = rows[-1]
1208     else:
1209       no_improve += 1
1210
1211     if no_improve >= PATIENCE_DMDC:
1212       print(f"[EARLY STOP] DMDC Grid no improvement for PATIENCE_DMDC={PATIENCE_DMDC} trials.")
1213       break
1214
1215   except Exception as e:
1216     rows.append(dict(
1217       score=np.inf,
1218       r_omega=rO, tik=tik, rho_max=rho_max, clip=clip,
1219       hankel_d=d_h, hankel_rank=r_h, hankel_tik=htik, hankel_rho=hrho,
1220       hankel_clip=hclip,
1221       run_dir=run_dir, error=str(e)
1222     ))
1223     no_improve += 1
1224     if no_improve >= PATIENCE_DMDC:
1225       print(f"[EARLY STOP] DMDC Grid (errors/no improvement) hit PATIENCE_DMDC={PATIENCE_DMDC}.")
1226       break
1227
1228 df = pd.DataFrame(rows).sort_values("score").reset_index(drop=True)
1229 return df, best

```

```

1227
1228 def smart_expand_grid_dmdc(df_stage1):
1229     cands = _top_candidates(df_stage1, STAGE2_TOP_CANDIDATES)
1230     if not cands:
1231         return None
1232
1233     r0_list = []
1234     tik_list = []
1235     hankel_rank_list = []
1236     hankel_tik_list = []
1237     for c in cands:
1238         r0_list += _expand_rank(int(c["r_omega"]), STAGE2_NEIGHBOR_RANK, low=2, high=120)
1239         tik_list += _expand_tik(float(c["tik"]), STAGE2_MULTIPLIERS_TIK)
1240         hankel_rank_list += _expand_rank(int(c["hankel_rank"]), STAGE2_NEIGHBOR_RANK, low=10, high=300)
1241         hankel_tik_list += _expand_tik(float(c["hankel_tik"]), STAGE2_MULTIPLIERS_TIK)
1242
1243     GRID2 = dict(
1244         DMDC_RANK_OMEGA_GRID=sorted(set(r0_list)),
1245         DMDC_TIK_GRID=unique_sorted(tik_list),
1246         DMDC_RHO_MAX_GRID=[0.995],
1247         DMDC_CLIP_GRID=[None],
1248
1249         DMDC_HANKEL_D_GRID=[16],
1250         DMDC_HANKEL_RANK_GRID=sorted(set(hankel_rank_list)),
1251         DMDC_HANKEL_TIK_GRID=unique_sorted(hankel_tik_list),
1252         DMDC_HANKEL_RHO_MAX_GRID=[0.995],
1253         DMDC_HANKEL_CLIP_GRID=[None],
1254     )
1255     return GRID2
1256
1257 # =====
1258 # ☑ NEW: ML (LR + RF) comparison for 1-year horizon
1259 # One-step formulation:
1260 #     input_k = [x_state(k); u(k)] -> target = x_state(k+1)
1261 # =====
1262
1263 def ml_train_test_one_year(X_state, U_ctrl, state_names, ctrl_names, time_cols,
1264 out_dir):
1265     """
1266     Compare ML baselines: Random Forest (RF) and Linear Regression (LR).
1267     - Performance evaluation
1268     - Visualization (Real vs Pred, error curves)
1269     """
1270     ensure_dir(out_dir)
1271
1272     try:
1273         from sklearn.linear_model import LinearRegression
1274         from sklearn.ensemble import RandomForestRegressor
1275         from sklearn.multioutput import MultiOutputRegressor
1276     except Exception as e:
1277         print("[WARN] scikit-learn not available. ML comparison skipped. Error:", e)
1278         return None
1279
1280     X_state = np.asarray(X_state, float)
1281     U_ctrl = np.asarray(U_ctrl, float)
1282     n, T = X_state.shape
1283     p, Tu = U_ctrl.shape
1284     if Tu != T:
1285         raise ValueError("U_ctrl length must match X_state length for ML compare.")
1286
1287     # Supervised dataset:
1288     # features at k: [x(k), u(k)] ; target: x(k+1)
1289     Xk = X_state[:, :-1].T # (T-1, n)
1290     Uk = U_ctrl[:, :-1].T # (T-1, p)
1291     F = np.hstack([Xk, Uk]) # (T-1, n+p)
1292     Y = X_state[:, 1:].T # (T-1, n)
1293
1294     total = F.shape[0]
1295     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) >= T else [f"t{i}" for i in range(1, T)]
1311     time_te = time_for_targets[train_n:train_n + test_n]
1312
1313     # Models
1314     lr = MultiOutputRegressor(LinearRegression())
1315     rf = MultiOutputRegressor(RandomForestRegressor(
1316         n_estimators=RF_N_ESTIMATORS,
1317         random_state=ML_RANDOM_STATE,
1318         n_jobs=-1,
1319         max_depth=RF_MAX_DEPTH,
1320         min_samples_leaf=RF_MIN_SAMPLES_LEAF
1321     ))
1322
1323     # Fit
1324     lr.fit(F_tr, Y_tr)
1325     rf.fit(F_tr, Y_tr)
1326
1327     # Predict (one-step)
1328     Y_lr = lr.predict(F_te)    # (test_n, n)
1329     Y_rf = rf.predict(F_te)
1330
1331     # Convert to (n, test_n)
1332     X_true_year = Y_te.T
1333     X_lr_year = np.asarray(Y_lr, float).T
1334     X_rf_year = np.asarray(Y_rf, float).T
1335
1336     # Metrics
1337     df_lr, score_lr = metrics_rowwise(X_true_year, X_lr_year, state_names)
1338     df_rf, score_rf = metrics_rowwise(X_true_year, X_rf_year, state_names)
1339
1340     # Plots
1341     if SAVE_PLOTS:
1342         plot_ml_compare_one_year(time_te, X_true_year, X_lr_year, state_names, "LR",
1343                                   out_dir)
1344         plot_ml_compare_one_year(time_te, X_true_year, X_rf_year, state_names, "RF",
1345                                   out_dir)
1346
1347     return dict(
1348         test_n=test_n,
1349         train_n=train_n,
1350         time_te=time_te,
1351         X_true_year=X_true_year,
1352         X_lr_year=X_lr_year,
1353         X_rf_year=X_rf_year,
1354         met_lr=df_lr, score_lr=score_lr,
1355         met_rf=df_rf, score_rf=score_rf
1356     )
1357
1358     # =====
1359     # MAIN
1360     # =====
1361
1362     if __name__ == "__main__":
1363         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,
1367           "Spike-hybrid:", USE_SPIKE_HYBRID)
1368
1369     # -----
1370     # PREPROCESS SELECTOR
1371     # -----
1372     if DO_CLEAN_NORMALIZE:
1373         if USE_PIPELINE_1_9:
1374             df_use = preprocess_pipeline_1_9(
1375                 xlsx_path=XLSX_PATH,
1376                 sheet_name=TPYS_SHEET,
1377                 out_path=PIPELINE_1_9_OUT_PATH,
1378                 date_col_name=DATE_COL,
1379                 hour_col_name=HOUR_COL,
1380                 value_cols=TPYS_COLS_REQUIRED,
1381                 round_digits=5
1382             )
1383             print("[OK] Pipeline 1..9 saved to:", PIPELINE_1_9_OUT_PATH)
1384
1385     else:
1386         df_wide = build_df_wide_from_tpys(XLSX_PATH, TPYS_SHEET)
1387
1388         # log1p -> MinMax row-wise
1389         Xn_all, _, _ = log1p_minmax_rows(df_wide.values.astype(float))
1390         Xn_all = np.clip(Xn_all, 0.0, 1.0)
1391         df_wide_proc = pd.DataFrame(Xn_all, index=df_wide.index, columns=df_wide.columns)
1392
1393         with pd.ExcelWriter(PROSSESSED_WIDE_PATH, engine="openpyxl") as writer:
1394             df_wide_proc.to_excel(writer, sheet_name=PROSESSED_WIDE_SHEET)
1395
1396             print("[OK] Saved processed wide (log1p->MinMax ROW) to:",
1397                  PROSESSED_WIDE_PATH)
1398             df_use = df_wide_proc
1399
1400     else:
1401         df_use = build_df_wide_from_tpys(XLSX_PATH, TPYS_SHEET)
1402
1403     # -----
1404     # Build matrices
1405     # -----
1406
1407     X_dmd, dmd_names = pick_rows_from_dfwide(df_use, DMD_ROWS)
1408     X_state, state_names = pick_rows_from_dfwide(df_use, STATE_ROWS)
1409     U_ctrl, ctrl_names = pick_rows_from_dfwide(df_use, CONTROL_ROWS)
1410
1411     print("\n==== Shapes ====")
1412     print("X_dmd : ", X_dmd.shape)
1413     print("X_state: ", X_state.shape)
1414     print("U_ctrl : ", U_ctrl.shape)
1415     print("state rows:", state_names)
1416     print("ctrl rows :", ctrl_names)
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, dmddc_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_dmddc_df_s1 = None
1468 grid_dmddc_df_s2 = None
1469
1470 best_dmd = None
1471 best_dmddc = None
1472
# ---- Grid Search ----
1473 if CALIBRATION_MODE == "auto":
1474     print("\n>> GRID SEARCH STAGE-1: DMD + Hankel")
1475     grid_dmd_df_s1, best_dmd = grid_search_dmd_hankel(X_dmd, dmd_names, stage_name
1476 = "S1")
1477     print(grid_dmd_df_s1.head(GRID["TOP_K"]))
1478
1479     print("\n>> GRID SEARCH STAGE-1: DMDC + Hankel")
1480     grid_dmddc_df_s1, best_dmddc = grid_search_dmddc_hankel(X_state, U_ctrl,
1481                                               state_names, ctrl_names, stage_name="S1")
1482     print(grid_dmddc_df_s1.head(GRID["TOP_K"]))
1483
1484 if SMART_GRID and (not STAGE1_ONLY):
1485     GRID2_DMD = smart_expand_grid_dmd(grid_dmd_df_s1)
1486     if GRID2_DMD is not None:
1487         print("\n>> SMART EXPAND STAGE-2: DMD + Hankel (around best)")
1488         GRID_backup = GRID.copy()
1489         GRID.update(GRID2_DMD)
1490         grid_dmd_df_s2, best_dmd_s2 = grid_search_dmd_hankel(X_dmd, dmd_names,
1491                                               stage_name="S2")
1492         print(grid_dmd_df_s2.head(GRID["TOP_K"]))
1493         if best_dmd is None or (best_dmd_s2 is not None and best_dmd_s2[
1494             "score"] < best_dmd["score"]):
1495             best_dmd = best_dmd_s2
1496             GRID = GRID_backup
1497
1498 GRID2_DMDC = smart_expand_grid_dmddc(grid_dmddc_df_s1)
1499 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_dmdc is not None:  

1508         print("\n\x25 BEST DMD+Hankel:", best_dmdc)  

1509     if best_dmdc is not None:  

1510         print("\n\x25 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     # \x25 NEW: ML comparison (RF + LR) on 1-year window
1564     # =====
1565     ml_pack = None
1566     if ENABLE_COMPARE:

```

```

1564
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
1567         None
1568     ml_pack = ml_train_test_one_year(X_state, U_ctrl, state_names, ctrl_names,
1569         time_cols, ml_dir)
1570     if ml_pack is not None:
1571         print("[OK] ML comparison finished. LR score:", ml_pack["score_lr"],
1572             "RF score:", ml_pack["score_rf"])
1573     except Exception as e:
1574         print("[WARN] ML comparison failed:", e)
1575         ml_pack = None
1576
1577 # -----
1578 # EXPORT (metrics + grids + summary + REQUESTED MATRICES)
1579 # -----
1580 with pd.ExcelWriter(OUT_XLSX, engine="openpyxl") as writer:
1581
1582     # --- Metrics sheets ---
1583     if results.get("DMD_manual") is not None:
1584         results["DMD_manual"]["met_dmd"].to_excel(writer, sheet_name=
1585             "DMD_manual_metrics", index=False)
1586         results["DMD_manual"]["met_h"].to_excel(writer, sheet_name=
1587             "HankelDMD_metrics", index=False)
1588
1589     if results.get("DMDC_manual") is not None:
1590         results["DMDC_manual"]["met_c"].to_excel(writer, sheet_name=
1591             "DMDC_manual_metrics", index=False)
1592         results["DMDC_manual"]["met_h"].to_excel(writer, sheet_name=
1593             "HankelDMDC_metrics", index=False)
1594
1595     if results.get("DMDC_best_replot") is not None:
1596         results["DMDC_best_replot"]["met_h"].to_excel(writer, sheet_name=
1597             "BEST_DMDC_H_metrics", index=False)
1598
1599     # --- ML metrics ---
1600     if ml_pack is not None:
1601         ml_pack["met_lr"].to_excel(writer, sheet_name="ML_LR_metrics", index=False)
1602         ml_pack["met_rf"].to_excel(writer, sheet_name="ML_RF_metrics", index=False)
1603
1604     # --- Grid sheets ---
1605     if grid_dmd_df_s1 is not None:
1606         grid_dmd_df_s1.to_excel(writer, sheet_name="GRID_DMD_S1", index=False)
1607     if grid_dmd_df_s2 is not None:
1608         grid_dmd_df_s2.to_excel(writer, sheet_name="GRID_DMD_S2", index=False)
1609
1610     if grid_dmdc_df_s1 is not None:
1611         grid_dmdc_df_s1.to_excel(writer, sheet_name="GRID_DMDC_S1", index=False)
1612     if grid_dmdc_df_s2 is not None:
1613         grid_dmdc_df_s2.to_excel(writer, sheet_name="GRID_DMDC_S2", index=False)
1614
1615     # --- Summary ---
1616     summary = []
1617     if results.get("DMD_manual") is not None:
1618         summary.append(dict(model="Affine_DMD_manual_Hankel", score=results[
1619             "DMD_manual"]["score_h"], run_dir=os.path.join(FIG_ROOT, "DMD_MANUAL")))
1620     if results.get("DMDC_manual") is not None:
1621         summary.append(dict(model="Affine_DMDC_manual_Hankel", score=results[
1622             "DMDC_manual"]["score_h"], run_dir=os.path.join(FIG_ROOT, "DMDC_MANUAL")))
1623     if best_dmd is not None:
1624         summary.append(dict(model="DMD_grid_best", score=best_dmd["score"],
1625             run_dir=best_dmd["run_dir"]))
1626     if best_dmddc is not None:
1627         summary.append(dict(model="DMDC_grid_best", score=best_dmddc["score"],
1628             run_dir=best_dmddc["run_dir"]))
1629     if results.get("DMDC_best_replot") is not None:
1630         summary.append(dict(model="DMDC_best_replot", score=results[
1631             "DMDC_best_replot"]["score_h"], run_dir=os.path.join(FIG_ROOT,
1632                 "BEST_DMDC_REPLOT")))

```

```

1619
1620     if ml_pack is not None:
1621         summary.append(dict(model="ML_LR_1year", score=ml_pack["score_lr"]),
1622                         run_dir=os.path.join(FILE_ROOT, "ML_RF_LR_1YEAR")))
1623         summary.append(dict(model="ML_RF_1year", score=ml_pack["score_rf"]),
1624                         run_dir=os.path.join(FILE_ROOT, "ML_RF_LR_1YEAR")))
1625     pd.DataFrame(summary).to_excel(writer, sheet_name="SUMMARY", index=False)
1626
1627     # -----
1628     #  REQUESTED: save matrices (each in its own sheet)
1629     # -----
1630     col_names = list(df_use.columns) if isinstance(df_use, pd.DataFrame) else None
1631
1632     # -----
1633     # DMD exports
1634     # -----
1635     if results.get("DMD_manual") is not None:
1636         pack = results["DMD_manual"]
1637
1638         df_from_matrix(pack["X_real"], row_names=dmd_names, col_names=col_names).
1639             to_excel(writer, sheet_name="DMD_X_real")
1640         df_from_matrix(pack["X1_real"], row_names=dmd_names, col_names=(col_names
1641             [-1] if col_names else None)).to_excel(writer, sheet_name="DMD_X1")
1642         df_from_matrix(pack["X2_real"], row_names=dmd_names, col_names=(col_names[1:]
1643             if col_names else None)).to_excel(writer, sheet_name="DMD_X2")
1644
1645         # Normalized
1646         df_from_matrix(pack["Xn"], row_names=dmd_names, col_names=col_names).
1647             to_excel(writer, sheet_name="DMD_Xn_0_1")
1648         df_from_matrix(pack["Xdmd_n"], row_names=dmd_names, col_names=col_names).
1649             to_excel(writer, sheet_name="DMD_Xdmd_n_0_1")
1650         df_from_matrix(pack["Xhan_n"], row_names=dmd_names, col_names=col_names).
1651             to_excel(writer, sheet_name="DMD_Xhan_n_0_1")
1652
1653         # Real-space affine outputs
1654         df_from_matrix(pack["Xdmd"], row_names=dmd_names, col_names=col_names).
1655             to_excel(writer, sheet_name="DMD_Xaffine_dmd")
1656         df_from_matrix(pack["Xhan"], row_names=dmd_names, col_names=col_names).
1657             to_excel(writer, sheet_name="DMD_Xaffine_dmd_H")
1658
1659         # A, b (and Hankel Ah, bh)
1660         if pack.get("A") is not None:
1661             df_from_square(pack["A"], names=dmd_names).to_excel(writer, sheet_name
1662                 ="DMD_A")
1663             if pack.get("b") is not None:
1664                 df_from_vector(pack["b"], row_names=dmd_names, col_name="b").to_excel(
1665                     writer, sheet_name="DMD_b")
1666             if pack.get("Ah") is not None:
1667                 df_from_matrix(pack["Ah"]).to_excel(writer, sheet_name=safe_sheet_name
1668                     ("DMD_Ah_hankel"))
1669             if pack.get("bh") is not None:
1670                 df_from_vector(pack["bh"], col_name="bh").to_excel(writer, sheet_name=
1671                     safe_sheet_name("DMD_bh_hankel"))
1672
1673         # -----
1674         # DMDC exports
1675         # -----
1676         if results.get("DMDC_manual") is not None:
1677             pack = results["DMDC_manual"]
1678
1679             df_from_matrix(pack["X_real"], row_names=state_names, col_names=col_names
1680                 ).to_excel(writer, sheet_name="DMDC_X_real")
1681             df_from_matrix(pack["X1_real"], row_names=state_names, col_names=(col_names
1682                 [-1] if col_names else None)).to_excel(writer, sheet_name="DMDC_X1")
1683             df_from_matrix(pack["X2_real"], row_names=state_names, col_names=(col_names[1:]
1684                 if col_names else None)).to_excel(writer, sheet_name="DMDC_X2")
1685
1686             # Normalized
1687             df_from_matrix(pack["Xn"], row_names=state_names, col_names=col_names).
1688                 to_excel(writer, sheet_name="DMDC_Xn_0_1")

```

```

1670 df_from_matrix(pack["Un"], row_names=ctrl_names, col_names=col_names).
1671     .to_excel(writer, sheet_name="DMDC_Un_0_1")
1672 df_from_matrix(pack["Xrec_n"], row_names=state_names, col_names=col_names)
1673     .to_excel(writer, sheet_name="DMDC_Xrec_n_0_1")
1674 df_from_matrix(pack["Xh_n"], row_names=state_names, col_names=col_names).
1675     .to_excel(writer, sheet_name="DMDC_Xh_n_0_1")
1676
1677 # Real-space affine outputs
1678 df_from_matrix(pack["Xrec"], row_names=state_names, col_names=col_names).
1679     .to_excel(writer, sheet_name="DMDC_Xaffine_dmdc")
1680 df_from_matrix(pack["Xh"], row_names=state_names, col_names=col_names).
1681     .to_excel(writer, sheet_name="DMDC_Xaffine_dmdc_H")
1682
1683 # A, B, b (and Hankel Ah, Bh, bh)
1684 if pack.get("A") is not None:
1685     df_from_square(pack["A"], names=state_names).to_excel(writer,
1686         sheet_name="DMDC_A")
1687 if pack.get("B") is not None:
1688     df_from_matrix(pack["B"], row_names=state_names, col_names=ctrl_names
1689         ).to_excel(writer, sheet_name="DMDC_B")
1690 if pack.get("b") is not None:
1691     df_from_vector(pack["b"], row_names=state_names, col_name="b").
1692         to_excel(writer, sheet_name="DMDC_b")
1693
1694 if pack.get("Ah") is not None:
1695     df_from_matrix(pack["Ah"]).to_excel(writer, sheet_name=safe_sheet_name
1696         ("DMDC_Ah_hankel"))
1697 if pack.get("Bh") is not None:
1698     df_from_matrix(pack["Bh"]).to_excel(writer, sheet_name=safe_sheet_name
1699         ("DMDC_Bh_hankel"))
1700 if pack.get("bh") is not None:
1701     df_from_vector(pack["bh"], col_name="bh").to_excel(writer, sheet_name=
1702         safe_sheet_name("DMDC_bh_hankel"))
1703
1704 # -----
1705 # ML exports (1-year window)
1706 # -----
1707 if ml_pack is not None:
1708     te_cols = ml_pack["time_te"]
1709     df_from_matrix(ml_pack["X_true_year"], row_names=state_names, col_names=
1710         te_cols).to_excel(writer, sheet_name="ML_TRUE_1Y")
1711     df_from_matrix(ml_pack["X_lr_year"], row_names=state_names, col_names=
1712         te_cols).to_excel(writer, sheet_name="ML_LR_PRED_1Y")
1713     df_from_matrix(ml_pack["X_rf_year"], row_names=state_names, col_names=
1714         te_cols).to_excel(writer, sheet_name="ML_RF_PRED_1Y")
1715
1716     e_lr = rmse_over_time(ml_pack["X_true_year"], ml_pack["X_lr_year"])
1717     e_rf = rmse_over_time(ml_pack["X_true_year"], ml_pack["X_rf_year"])
1718     pd.DataFrame({"time": te_cols, "RMSE_over_states": e_lr}).to_excel(writer,
1719         sheet_name="ML_LR_ERR_1Y", index=False)
1720     pd.DataFrame({"time": te_cols, "RMSE_over_states": e_rf}).to_excel(writer,
1721         sheet_name="ML_RF_ERR_1Y", index=False)
1722
1723 print("\n[OK] Saved:", OUT_XLSX)
1724 print("[OK] Figures in:", FIG_ROOT)
1725
1726 if best_dmdc is not None:
1727     print("\nBest DMDc folder:", best_dmdc["run_dir"])
1728     try:
1729         os.startfile(best_dmdc["run_dir"])
1730     except Exception:
1731         pass
1732
1733 # =====
1734 # 📈 CALIBRATION / TUNING GUIDE (NUMBERED)
1735 # =====
1736 # [P01] DATA_DIR:           Change your workspace folder path.
1737 # [P02] XLSX_NAME:          Change your input Excel filename.
1738 # [P03] TPYS_SHEET:         Change the TPYS sheet name.
1739 # [P04]-[P05] Preprocessing selector: only ONE must be True.
1740 # [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
```