Machine Learning Introduction

BSAD 8310: Business Forecasting — Lecture 7

Department of Economics
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Why ML for Forecasting?

Classical methods are powerful — but structured. What happens when the structure breaks?

Six lectures built a powerful toolkit. Now we stress-test its assumptions.

What we have (L01–L06):

- Benchmarks and regression (L01–L02)
- ETS for trend + seasonality (L03)
- ARIMA/SARIMA for autocorrelation (L04)
- VAR, ARIMAX, ECM for multivariate dynamics (L05)
- Rigorous walk-forward evaluation (L06)

Classical models assume: linearity, fixed lag structure, Gaussian errors, known seasonality. When these fail, **model misspecification** inflates forecast error beyond what better data could fix.

Socratic: which assumption fails first when forecasting social-media-driven demand spikes for a new product?

Gap	Classical limit	ML remedy
Non-linearity	Linear $f(x)$ assumed	Trees, nets
Many predictors	VAR fails ($p > T$)	Regularization
Interactions	Hand-specified only	Learned
Non-Gaussian	Normality assumed	Distribution-free

ML does **not** replace ARIMA. It extends the toolkit for problems where: (1) predictors number in the hundreds, (2) relationships are non-linear, or (3) structure is unknown *a priori*.

(Hastie et al. 2009): the statistical learning perspective on non-linearity and interactions.

100,000 time series, 61 methods (Makridakis et al. 2020): nine of the top twelve methods were *hybrid* (classical + ML).

Method	Rank	sMAPE
Hybrid ES-RNN (ML + ETS)	1	11.37
Theta (classical)	2	11.37
FFORMA (ML ensemble)	3	11.57
Naive 2 (seasonal)	12	13.56
Auto ARIMA	14	13.58

Retail, electricity, and supply-chain forecasting now routinely use gradient-boosted trees and ensemble combinations of ARIMA + ML.

But: pure ML often *underperforms* naive on short series ($n < 100$). Context matters.

The Bias-Variance Tradeoff

Every modelling decision shifts error between bias and variance. This is the central tension in all of statistical learning.

2009

Let $\hat{f}$ be an estimated model and f the true function. At a new point x_0:

$$\mathrm{MSE}(\hat{f}(x_0)) = \left(\mathrm{Bias}[\hat{f}(x_0)]\right)^2 + \mathrm{Var}[\hat{f}(x_0)] + \sigma^2$$

σ^2 = irreducible noise (no model eliminates this).

- **Bias²**: systematic error from wrong model class (underfitting)
- **Variance**: sensitivity to particular training sample (overfitting)
- σ^2: irreducible — better models cannot reduce this, only better data can

$\hat{f}$: estimated model. f: true unknown function. x_0: feature vector at new observation. $\sigma^2 = \mathrm{Var}[\varepsilon]$ where ε is the noise term.

Both extremes hurt.

AR(1) fit to a threshold non-linear series: the model systematically underestimates peaks and overestimates troughs every cycle.

Low variance: refit on any subsample and the errors look the same.

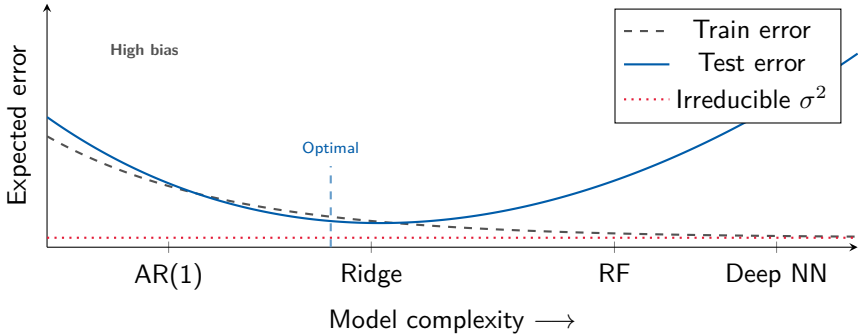
High variance — overfitting:

Degree-15 polynomial fits every wiggle in the training set. Train RMSE ≈ 0.02. Test RMSE $\approx 8\times$ train RMSE.

Small change in training data $\Rightarrow$ large change in $\hat{f}$.

Reducing bias *typically* increases variance. We control the tradeoff via **model complexity** and **regularization**.

Train error always falls with complexity. Test error has a U-shape.



Cross-validation finds the optimal complexity point without ever touching the test set.

Model	Bias	Var.	Good when
AR(1)	High	Low	Long, stable series
ARIMA (auto)	Medium	Low–Med	General TS
Ridge (many X)	Med	Low	Many predictors
OLS (unregul.)	Low	High	$n \gg p$ only
Deep LSTM	Low	High	Very long series

For short series ($n < 200$):

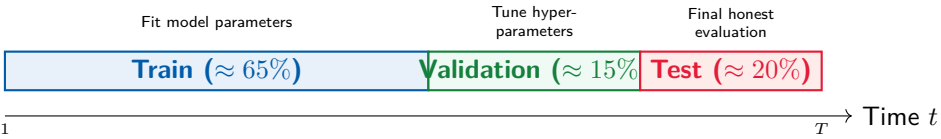
Bias is cheaper than variance.

Prefer parsimonious models. Add complexity only when cross-validation confirms out-of-sample improvement.

This directly motivates LASSO (L08): deliberately increasing bias via shrinkage to reduce variance on short, noisy series.

Train / Validation / Test Discipline

One split is not enough. Three sets, three roles — and the rules are strict.



Why three sets, not two?

If you tune on the test set — even once — it becomes a second validation set, and you no longer have an honest generalization estimate.

The test set is a **time capsule**. Open it exactly once, at the very end, to report the final number.

Leakage occurs when information from outside the training window contaminates the model, producing optimistic in-sample performance that does not generalize out-of-sample.

Feature leakage:

- Using next-month CPI to forecast this-month sales (future predictor)
- Target-encoding computed on the full dataset before splitting (statistical leakage)

Temporal leakage:

- Random train/test shuffle on a time series
- Fitting `StandardScaler` on the full series before splitting

Random train/test split is *correct* for i.i.d. data. It is **wrong** for time series. Always split in **chronological order**.

In production: leakage makes reported RMSE optimistic by $2\times$–$5\times$.

1. **No random shuffling** — always chronological order
2. **Validation after train, test after validation** — strict temporal ordering; no overlaps
3. **No future-dependent features** — any feature using time $t + k$ data cannot be known at time t
4. **Scale within each fold** — fit `StandardScaler` on train-fold only; transform val/test with train parameters
5. **Optional gap** — buffer between train end and val start prevents autocorrelation bleed-through

These rules are the time-series extensions of the bias-variance discipline.

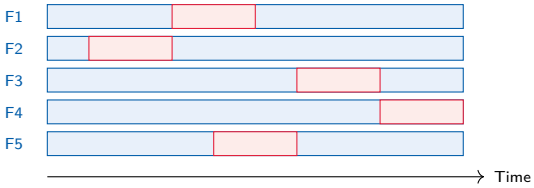
Break them and every accuracy number you report is invalid.

`train_test_split(shuffle=False)` respects ordering. Use `TimeSeriesSplit` for CV.

Cross-Validation for Time Series

Standard k-fold CV violates time ordering. Walk-forward CV is the fix.

Standard 5-fold (shuffled):



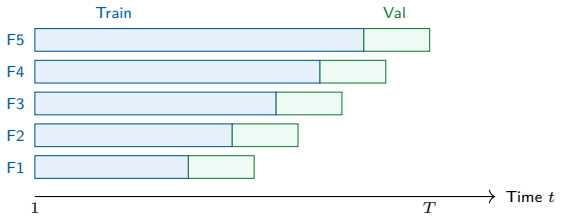
Wrong for time series: validation block may precede some training data $\Rightarrow$ temporal leakage.

Failure modes:

- Uses future data to predict the past
- Train and validation observations are not exchangeable under autocorrelation
- Validation RMSE is optimistically biased

Bergmeir et al. (2018): random k-fold gives biased CV estimates for autoregressive series. The bias grows with autocorrelation strength.

The correct analog: expanding-window validation introduced in L06, now applied to hyperparameter tuning.




```
from sklearn.model_selection import TimeSeriesSplit
tscv = TimeSeriesSplit(n_splits=5, gap=0)
for train_idx, val_idx in tscv.split(X):
    X_train, X_val = X[train_idx], X[val_idx]
```

gap: skip observations between train end and val start. Set gap=H when forecasting H steps ahead to prevent overlap.

General CV theory: (Arlot and Celisse 2010).

1. Choose candidate values:
   $\lambda \in \{0.01, 0.1, 1, 10, 100\}$
2. For each λ: run `TimeSeriesSplit` CV, compute mean validation RMSE
3. Select λ^* minimising mean CV RMSE
4. **Refit on full train + val** with λ^*
5. Evaluate exactly once on held-out test set

Step 4 is critical: refit on all non-test data. Using the CV train-fold only wastes data.

5-fold `TimeSeriesSplit`:

$\lambda = 0.1 \Rightarrow$ CV RMSE $= 1{,}780$ (optimal)

$\lambda = 0.001$ (overfit): $1{,}890$

$\lambda = 100$ (underfit): $2{,}140$

Test RMSE with $\lambda^* = 0.1$: $1{,}620$.

Regularization Preview

When there are many predictors, unconstrained OLS overfits. Shrinkage is the solution. Full treatment: Lecture 8.

2009

$$\hat{\beta} = \arg\min_{\beta} \underbrace{\sum_{t=1}^{T} (y_t - \beta^\top x_t)^2}_{\text{OLS loss}} + \lambda \cdot P(\beta)$$

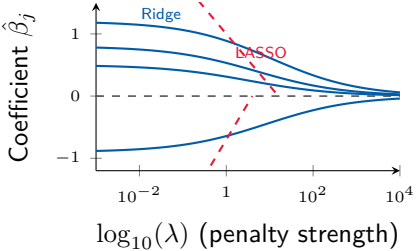
Ridge: $P(\beta) = \|\beta\|_2^2$ **LASSO (Tibshirani 1996):** $P(\beta) = \|\beta\|_1$ **EN (Zou and Hastie 2005):** $\alpha\|\beta\|_1 + (1-\alpha)\|\beta\|_2^2$

- **Ridge**: shrinks all coefficients smoothly; none reach exactly zero
- **LASSO**: sets some coefficients to exactly zero $\Rightarrow$ automatic variable selection
- **Elastic Net**: handles collinear predictors; ridge + LASSO combined

All three trade bias for variance via λ.

$\lambda = 0$: OLS (maximum variance).
$\lambda \to \infty$: intercept only (maximum bias).

Full derivation in L08.



As $\lambda \to \infty$: $\hat{\beta}_j \to 0$ (all predictors removed).

As $\lambda \to 0$: OLS solution.

LASSO paths hit zero at a finite λ — Ridge paths only approach zero asymptotically.

CV selects λ^* at the bias-variance minimum.

Illustrative paths. L08 derives the exact form from the subgradient conditions.

Feature Engineering Preview

ML models do not handle time series natively. We must create temporal structure explicitly.

Full treatment: Lecture 11.

A raw series $y_1, \ldots, y_T$ is not a feature matrix. We extract temporal patterns as columns.

Feature type	Formula	Business meaning
Lag	$x_t^{(k)} = y_{t-k}$	Sales k periods ago
Rolling mean	$\bar{y}_{t,w} = \frac{1}{w}\sum_{k=1}^{w} y_{t-k}$	Recent trend level
Rolling std	$s_{t,w} = \mathrm{std}(y_{t-w:t-1})$	Recent volatility
Month-of-year	$\mathbf{1}[\mathrm{month}(t) = m]$	Seasonal dummy
Trend counter	$t = 1, 2, \ldots, T$	Linear time trend

All features **must** use only $y_1, \ldots, y_{t-1}$ when predicting y_t. Any feature using y_t or later creates leakage. Apply `.shift(1)` before any rolling window.

Full treatment in L11: calendar features, Fourier terms, interaction features, and pipeline automation.

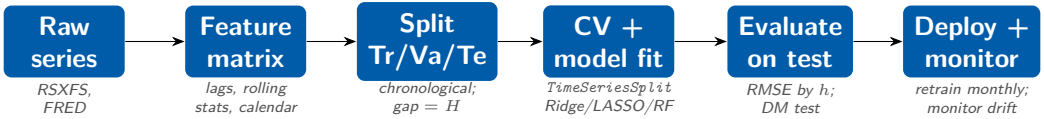
```python
# Lag features: shift(1) avoids leakage
X['lag_1']  = y.shift(1)
X['lag_12'] = y.shift(12)

# Rolling mean of y_{t-1}...y_{t-3}
X['roll_3'] = y.shift(1).rolling(3).mean
    ()

# Calendar feature (always known)
X['month'] = y.index.month

# Drop rows with NaN from lags
X = X.dropna()
```

- `.shift(1)`: shifts series forward one period — ensures x_t uses y_{t-1}, not y_t
- `.rolling(3).mean()` after `.shift(1)`: mean of $y_{t-1}, y_{t-2}, y_{t-3}$
- `.index.month`: calendar feature; no leakage (calendar is always known in advance)

L11 wraps this logic in a `sklearn.Pipeline` that prevents leakage automatically at every CV fold.

The ML Forecasting Pipeline

End-to-end: features $\rightarrow$ split $\rightarrow$ fit $\rightarrow$ evaluate $\rightarrow$ deploy.



The `sklearn.Pipeline` object chains preprocessing (`StandardScaler`) + model into a single estimator. This ensures the scaler is fitted on train-fold only during CV — eliminating a common source of leakage (James et al. 2021).

ML **extends** classical forecasting for non-linearity, many predictors, and unknown structure.

$\mathrm{MSE} = \mathrm{Bias}^2 + \mathrm{Var} + \sigma^2$ governs every modelling decision.

Three-way train/val/test split with chronological ordering is non-negotiable.

Walk-forward CV (`TimeSeriesSplit`) replaces k-fold for time series.

Regularization (L08) and feature engineering (L11) are the main levers for controlling bias-variance.

Lecture roadmap:

Lecture	Topic
L08	LASSO, Ridge, EN
L09	RF, XGBoost
L10	LSTM, attention
L11	Feature pipeline
L12	Capstone cases

Lab 7: full pipeline from raw RSXFS to LASSO and Ridge with walk-forward CV.

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- Bergmeir, Christoph, Rob J. Hyndman, and Bonsoo Koo (2018). "A Note on the Validity of Cross-Validation for Evaluating Autoregressive Time Series Prediction". In: *Computational Statistics & Data Analysis* 120, pp. 70–83.
- Hastie, Trevor, Robert Tibshirani, and Jerome Friedman (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. 2nd. New York: Springer. URL: `https://hastie.su.domains/ElemStatLearn/`.
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Tibshirani, Robert (1996). "Regression Shrinkage and Selection via the Lasso". In: *Journal of the Royal Statistical Society: Series B* 58.1, pp. 267–288.


Zou, Hui and Trevor Hastie (2005). "Regularization and Variable Selection via the Elastic Net". In: *Journal of the Royal Statistical Society: Series B* 67.2, pp. 301–320.