

# Theoretically Analysing Multi-Task Regression with Application to Time Series Forecasting

Romain Ilbert, Malik Tiomoko, Cosme Louart, Ambroise Odonnat, **Vasilii Feofanov**, Themis Palpanas, levgen Redko

Huawei Paris Noah's Ark Lab Paris Descartes University The Chinese University of Hong Kong

NeurIPS 2024, Spotlight NeurIPS @ Paris, December 5

#### Multivariate Time Series Forecasting









- Captures complex dependencies enhancing forecasting quality.
- Key for fields like economics, climate, and finance.
- Motivation of the paper: study it theoretically





- Modern forecasters are deep-learning-based.
- For theoretical derivations, we consider linear forecasting,





- Modern forecasters are deep-learning-based.
- For theoretical derivations, we consider linear forecasting,
- Or a deep model with a frozen feature extractor.

Our Framework: Multivariate as Multi-Task





• We view multivariate forecasting as a **multi-task** problem.

<sup>1</sup>(Xu et al., 2013) Multi-output least-squares support vector regression machines. 3

Our Framework: Multivariate as Multi-Task





• We view multivariate forecasting as a **multi-task** problem.

- Soft Parameter Sharing approach<sup>1</sup>:
  - $W_0$  catches the common part, reducing task overfitting.
  - $V_t$  are task-specific terms for individual biases.

<sup>&</sup>lt;sup>1</sup>(Xu et al., 2013) Multi-output least-squares support vector regression machines.



• **Problem Setup.** Time series channel  $t \in \{1, ..., T\}$  is viewed as a distinct task:

Training data:  $X^{(t)} \in \mathbb{R}^{d \times n_t}$ , Responses:  $Y^{(t)} \in \mathbb{R}^{q \times n_t}$ , d is seq. length, q is pred. horizon,  $n_t$  is sample size



• **Problem Setup.** Time series channel  $t \in \{1, ..., T\}$  is viewed as a distinct task:

Training data:  $X^{(t)} \in \mathbb{R}^{d \times n_t}$ , Responses:  $Y^{(t)} \in \mathbb{R}^{q \times n_t}$ , d is seq. length, q is pred. horizon,  $n_t$  is sample size

Linear Signal-Plus-Noise Model:

$$\mathbf{Y}^{(t)} = rac{{\mathbf{X}^{(t)}}^{ op} \mathbf{W}_t}{\sqrt{Td}} + \boldsymbol{\epsilon}^{(t)}, \quad \forall t,$$

- $\epsilon^{(t)}$  is noise,
- $W_t = W_0 + V_t$  combines shared  $W_0$  and task-specific components  $V_t$ :



$$\min \frac{1}{2\lambda} \|\boldsymbol{W}_{0}\|_{F}^{2} + \frac{1}{2} \sum_{t=1}^{T} \frac{\|\boldsymbol{V}_{t}\|_{F}^{2}}{\gamma_{t}} + \frac{1}{2} \sum_{t=1}^{T} \left\|\boldsymbol{Y}^{(t)} - \frac{\boldsymbol{X}^{(t)^{\top}} \boldsymbol{W}_{t}}{\sqrt{Td}}\right\|_{F}^{2}$$

•  $\lambda$  controls impact of the common part on a final prediction.



$$\min \frac{1}{2\lambda} \|\boldsymbol{W}_{0}\|_{F}^{2} + \frac{1}{2} \sum_{t=1}^{T} \frac{\|\boldsymbol{V}_{t}\|_{F}^{2}}{\gamma_{t}} + \frac{1}{2} \sum_{t=1}^{T} \left\|\boldsymbol{Y}^{(t)} - \frac{\boldsymbol{X}^{(t)}^{\top} \boldsymbol{W}_{t}}{\sqrt{Td}}\right\|_{F}^{2}$$

- $\lambda$  controls impact of the common part on a final prediction.
- $\gamma_t$  controls overfitting strength to the task t.



$$\min \frac{1}{2\lambda} \|\boldsymbol{W}_{0}\|_{F}^{2} + \frac{1}{2} \sum_{t=1}^{T} \frac{\|\boldsymbol{V}_{t}\|_{F}^{2}}{\gamma_{t}} + \frac{1}{2} \sum_{t=1}^{T} \left\|\boldsymbol{Y}^{(t)} - \frac{\boldsymbol{X}^{(t)}^{\top} \boldsymbol{W}_{t}}{\sqrt{Td}}\right\|_{F}^{2}$$

- $\lambda$  controls impact of the common part on a final prediction.
- $\gamma_t$  controls overfitting strength to the task t.
- Closed-form solution.



$$\min \frac{1}{2\lambda} \|\boldsymbol{W}_{0}\|_{F}^{2} + \frac{1}{2} \sum_{t=1}^{T} \frac{\|\boldsymbol{V}_{t}\|_{F}^{2}}{\gamma_{t}} + \frac{1}{2} \sum_{t=1}^{T} \left\|\boldsymbol{Y}^{(t)} - \frac{\boldsymbol{X}^{(t)^{\top}} \boldsymbol{W}_{t}}{\sqrt{Td}}\right\|_{F}^{2}$$

- $\lambda$  controls impact of the common part on a final prediction.
- $\gamma_t$  controls overfitting strength to the task t.
- Closed-form solution.

#### Questions:

- What are generalization guarantees of the model?
- How to balance the shared and task-specific components?

• Traditional: d is fixed, n is large  $(n \gg d, n \rightarrow \infty)$ .



- Traditional: d is fixed, n is large  $(n \gg d, n \rightarrow \infty)$ .
- Small-data: n is small, d is large,  $(n \ll d, d \rightarrow \infty)$ .

## Random Matrix Analysis

Three types of asymptotic analysis:

- Traditional: d is fixed, n is large  $(n \gg d, n \rightarrow \infty)$ .
- Small-data: n is small, d is large,  $(n \ll d, d \rightarrow \infty)$ .
- Large-dimensional: n, d are both large  $(c_0 = \frac{d}{n} = \mathcal{O}(1), (n, d) \rightarrow \infty)$ .





- Traditional: d is fixed, n is large  $(n \gg d, n \rightarrow \infty)$ .
- Small-data: n is small, d is large,  $(n \ll d, d \rightarrow \infty)$ .

• Large-dimensional: n, d are both large  $(c_0 = \frac{d}{n} = \mathcal{O}(1), (n, d) \rightarrow \infty)$ .

Assumptions on data distribution:

Noise is randomly sampled from a fixed distribution with 0-mean and covariance  $\Sigma_N \in \mathbb{R}^{q \times q}$ .



- Traditional: d is fixed, n is large  $(n \gg d, n \rightarrow \infty)$ .
- Small-data: n is small, d is large,  $(n \ll d, d \rightarrow \infty)$ .

■ Large-dimensional: n, d are both large  $(c_0 = \frac{d}{n} = \mathcal{O}(1), (n, d) \rightarrow \infty)$ .

Assumptions on data distribution:

- Noise is randomly sampled from a fixed distribution with 0-mean and covariance  $\Sigma_N \in \mathbb{R}^{q \times q}$ .
- Concentrated Data (Louart, C. and Couillet, R., 2018): variance of  $\mathbf{x}^{\top} \mathbf{W}_t$  does not grow with dimension d,





- Traditional: d is fixed, n is large  $(n \gg d, n \rightarrow \infty)$ .
- Small-data: n is small, d is large,  $(n \ll d, d \rightarrow \infty)$ .

■ Large-dimensional: n, d are both large  $(c_0 = \frac{d}{n} = \mathcal{O}(1), (n, d) \rightarrow \infty)$ .

Assumptions on data distribution:

Noise is randomly sampled from a fixed distribution with 0-mean and covariance  $\Sigma_N \in \mathbb{R}^{q \times q}$ .

• Concentrated Data (Louart, C. and Couillet, R., 2018): variance of  $\mathbf{x}^{\top} \mathbf{W}_t$  does not grow with dimension d, Particular cases:

- Standard Gaussian distribution,
- Lipschitz transformation of Gaussian (e.g., GAN images),
- Open question: features learned by DNN?





We want to evaluate the asymptotic train and test risk:

$$\mathcal{R}_{train}^{\infty} = \frac{1}{Tn} \sum_{t=1}^{T} \mathbb{E}\left[ \| \boldsymbol{Y}^{(t)} - g(\boldsymbol{X}^{(t)}) \|_{2}^{2} \right], \quad \mathcal{R}_{test}^{\infty} = \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\| \boldsymbol{y}^{(t)} - g(\boldsymbol{x}^{(t)}) \|_{2}^{2}].$$

#### Theorem (Asymptotic Train and Test Risk)

Under the large-dimension regime and concentration assumption, the asymptotic train and test risks are explicitly derived, with analytical curves in closed form depending on the hyperparameters, signal-generating hyperplane, and noise level.

#### Sketch of Proof.

 Following the notion of deterministic equivalents of a random matrix, we compute for the test risk:

$$\mathbb{E}_{\mathbf{x},\mathbf{X}^{(t)}}\left[\|\mathbf{y}^{(t)}-\boldsymbol{\omega}^*(\mathbf{X}^{(t)})^{\top}\mathbf{x}\|_2^2\right],$$



For two tasks (T = 2) with identity covariance and  $\gamma_1 = \gamma_2 = \gamma$ , the asymptotic test risk simplifies to:

$$\mathcal{R}_{\mathsf{test}}^{\infty} = \underbrace{\boldsymbol{D}_{ST}(\|\boldsymbol{W}_1\|_2^2 + \|\boldsymbol{W}_2\|_2^2)}_{\textit{Signal Term}} + \underbrace{\boldsymbol{C}_{CTT}\boldsymbol{W}_1^\top\boldsymbol{W}_2}_{\textit{Cross-Task Term}} + \underbrace{\boldsymbol{N}_{NT}\operatorname{tr}\boldsymbol{\Sigma}_n}_{\textit{Noise Term}},$$

•  $D_{ST}$ ,  $C_{CTT}$  and  $N_{NT}$  are functions of  $\lambda$ ,  $\gamma$ , n and d.

For two tasks (T = 2) with identity covariance and  $\gamma_1 = \gamma_2 = \gamma$ , the asymptotic test risk simplifies to:

$$\mathcal{R}_{\mathsf{test}}^{\infty} = \underbrace{\boldsymbol{D}_{ST}(\|\boldsymbol{W}_1\|_2^2 + \|\boldsymbol{W}_2\|_2^2)}_{Signal \ Term} + \underbrace{\boldsymbol{C}_{CTT}\boldsymbol{W}_1^\top\boldsymbol{W}_2}_{Cross-Task \ Term} + \underbrace{\boldsymbol{N}_{NT} \operatorname{tr}\boldsymbol{\Sigma}_n}_{Noise \ Term},$$

**D**<sub>ST</sub>,  $C_{CTT}$  and  $N_{NT}$  are functions of  $\lambda$ ,  $\gamma$ , n and d.

Optimal balance between signal and noise terms:

$$\lambda^{\star} = \frac{n}{d} \left( \frac{\|\boldsymbol{W}_1\|_2^2 + \|\boldsymbol{W}_2\|_2^2}{\operatorname{tr} \boldsymbol{\Sigma}_N} + \frac{\boldsymbol{W}_1^{\top} \boldsymbol{W}_2}{\operatorname{tr} \boldsymbol{\Sigma}_N} \right) - \frac{\gamma}{2}.$$

Ilbert, Tiomoko, et al., by Feofanov



### Contribution of Each Term to Tesk Risk





- <u>Observations.</u> As lambda increases, the cross-term and signal term decrease, while the noise term increases.
- Explanation. A large lambda forces tasks to interact, leveraging their relationships (decreasing cross term) but risking to increase noise and create non-existent patterns.

## Theoretical vs Empirical Risk



#### Experimental Setup:

- Two-task setting (T = 2):  $W_1 \sim \mathcal{N}(0, I_d)$ ,  $W_2 = \alpha W_1 + \sqrt{1 - \alpha^2} W_1^{\perp}$ .
- $\alpha \in [0,1]$  controls task similarity,  $\pmb{W}_1^\perp$  is orthogonal to  $\pmb{W}_1.$

## Theoretical vs Empirical Risk

- Experimental Setup:
  - Two-task setting (T = 2):  $W_1 \sim \mathcal{N}(0, I_d), \quad W_2 = \alpha W_1 + \sqrt{1 - \alpha^2} W_1^{\perp}.$
  - $\alpha \in [0,1]$  controls task similarity,  $W_1^{\perp}$  is orthogonal to  $W_1$ .
- Results:
  - $\bullet$  We compare theoretical asymptotic error with empirical one by varying  $\lambda$  and  $\alpha.$
  - $\bullet\,$  Theoretical curves align well the empirical ones  $\Rightarrow$  potential for model selection.





- Idea: use multi-task loss to train univariate model for multivariate forecasting.
  - 3 Forecasters: PatchTST, DLinearU, Transformer.
  - 3 Multivariate SOTA: SAMformer, DLinearM, iTransformer.
  - $\lambda$  and  $\gamma_t$  are hyperopted.
- This easy trick to learn channel interactions improves all the 3 considered models.

Dataset	Н	with MTL regularization			without MTL regularization					
		PatchTST	DLinearU	Transformer	PatchTST	DLinearU	DLinearM	Transformer	SAMformer <sup>†</sup>	$iTransformer^{\dagger}$
ETTh1	96	0.385	0.367*	0.368	0.387	0.397	0.386	0.370	0.381	0.386
	192	0.422	0.405*	$0.407^{*}$	0.424	0.422	0.437	0.411	0.409	0.441
	336	$0.433^{*}$	0.431	0.433	0.442	0.431	0.481	0.437	0.423	0.487
	720	$0.430^{*}$	0.454	$0.455^{*}$	0.451	0.428	0.519	0.470	0.427	0.503
EITh2	96	0.291	$0.267^{*}$	0.270	0.295	0.294	0.333	0.273	0.295	0.297
	192	$0.346^{*}$	0.331*	0.337	0.351	0.361	0.477	0.339	0.340	0.380
	336	0.332*	0.367	$0.366^{*}$	0.342	0.361	0.594	0.369	0.350	0.428
	720	0.384*	0.412	$0.405^{*}$	0.393	0.395	0.831	0.428	0.391	0.427
Weather	96	0.148	0.149*	$0.154^{*}$	0.149	0.196	0.196	0.170	0.197	0.174
	192	0.190	$0.206^{*}$	$0.198^{*}$	0.193	0.243	0.237	0.214	0.235	0.221
	336	$0.242^{*}$	$0.249^{*}$	0.258	0.246	0.283	0.283	0.260	0.276	0.278
	720	0.316*	$0.326^{*}$	0.331	0.322	0.339	0.345	0.326	0.334	0.358

## Thank you for your attention!



Paper

Paris Noah's Ark Lab