TabPFN: One Model to Rule Them All?

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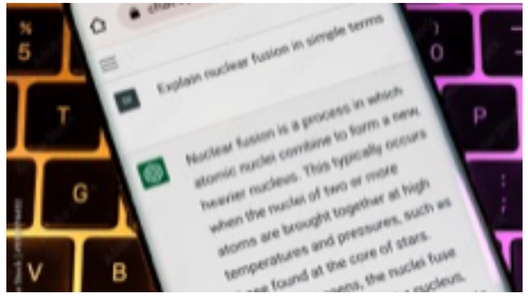
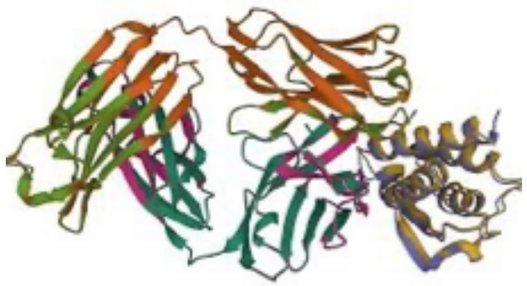
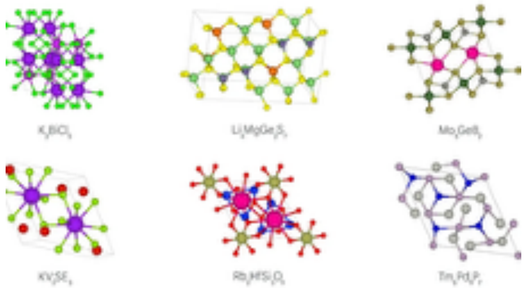
*Contributed equally

The deep learning revolution in data science

Deep learning has many successes, particularly in *computer vision* and *NLP*

	NLP/image generation	Biosciences	Material science
Past			
Present			
	Deepseek/ChatGPT	**AlphaFold**	**GNoME**

Old story: deep learning struggles with tabular data

	0	1	2
0	1.5	21.0	'Mia'
1	4.0	35.0	'Lucas'
2	3.0	17.0	'Ang'
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Numerical and string datatypes

Grinsztajn et al. (NeurIPS 2022) Why do tree-based models still outperform deep learning on typical tabular data?

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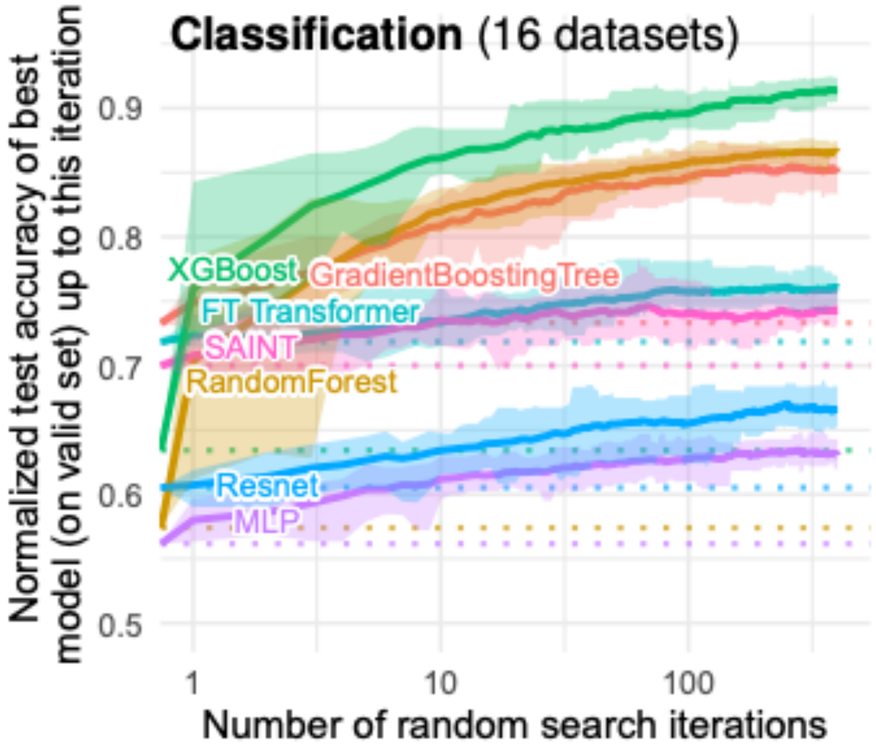
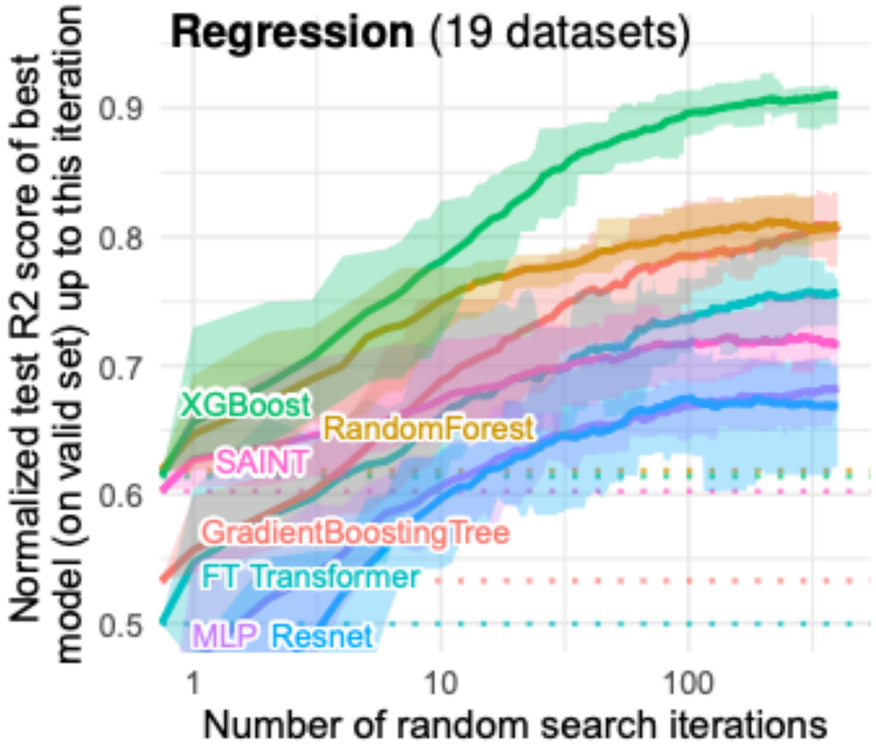
However, tree ensembles were gold standards for tabular data classification & regression





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Article

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Open access

Check for updates

Noah Hollmann[1,2,3,7]✉, Samuel Müller[1,7]✉, Lennart Purucker[1], Arjun Krishnakumar[1], Max Körfer[1], Shi Bin Hoo[1], Robin Tibor Schirrmeister[4,5] & Frank Hutter[1,3,6]✉

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A new breakthrough: deep learning outperforms tree ensembles

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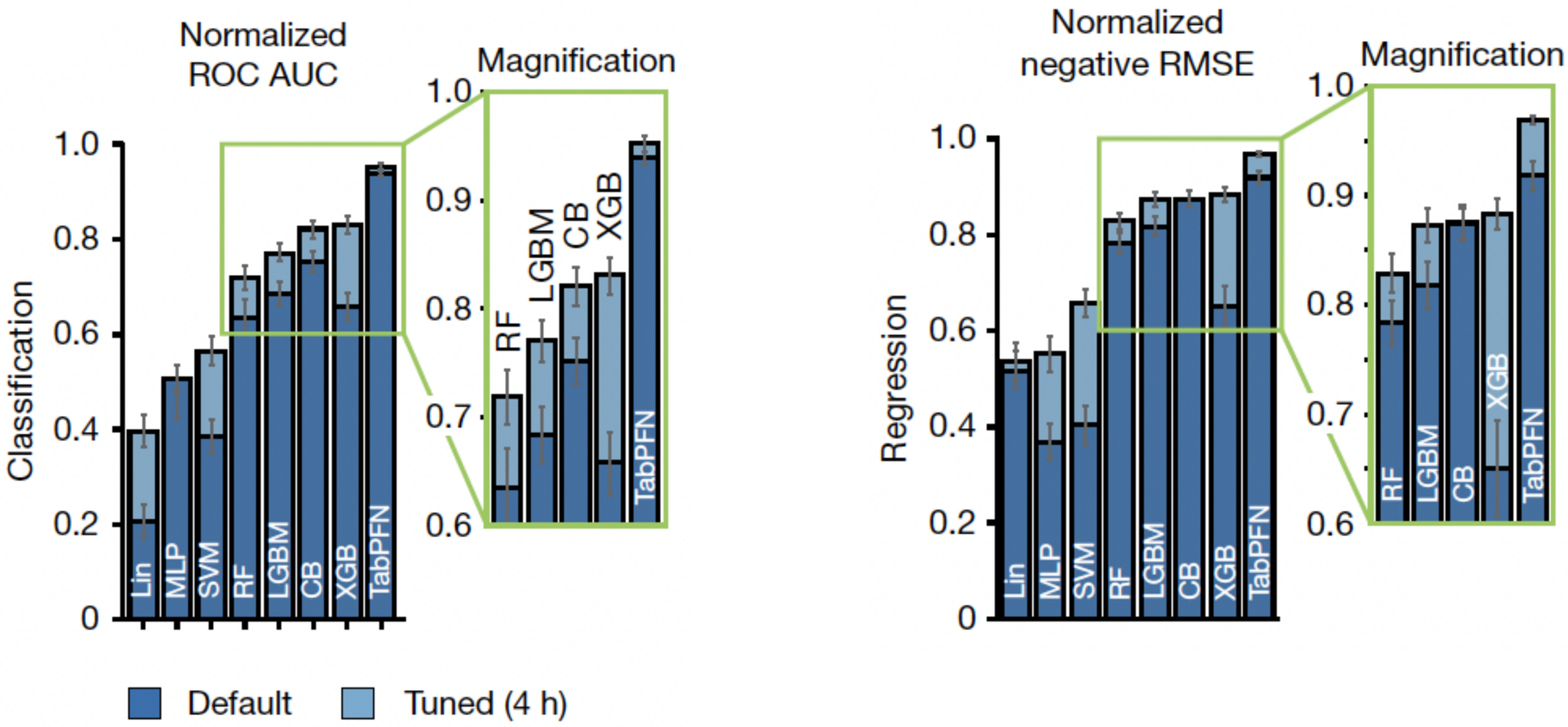

57 benchmark regression and classification datasets

TabPFN is a foundation model

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As a remedy, we introduce TabPFN, a foundation model for small- to medium-sized tabular data. This new supervised tabular learning method can be applied to any small- to moderate-sized dataset and yields dominant performance for datasets with up to 10,000 samples and 500 features. In a single forward pass, TabPFN significantly outperforms state-of-the-art baselines on our benchmarks, including gradient-boosted decision trees, even when these are allowed 4 h of tuning, a speedup of 5,140× (classification) and 3,000× (regression). Finally, we demonstrate various foundation model characteristics of TabPFN, including fine-tuning, generative abilities and density estimation.

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FM for tabular data

TabPFN

Goal of this talk

What is TabPFN?

Explain TabPFN from a statistical perspective

Is it good for statistical estimation?

Case studies: semi-supervised parameter estimation, heterogeneous treatment effects estimation, ~~prediction under covariate shift~~

Why does TabPFN work so well?

TabPFN's adaptivity on specific structures

How TabPFN works?

In-context learning

In-context learning (ICL): a technique where pre-trained LLMs learn new tasks from a few examples in the form of prompt, without requiring fine-tuning or parameter updates.

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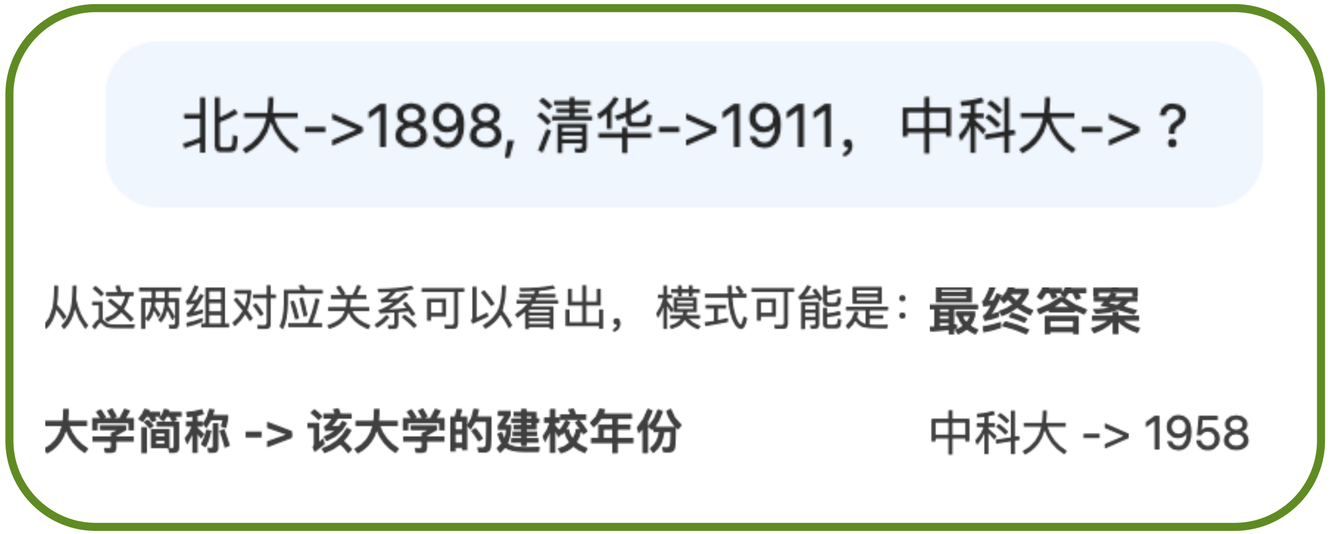

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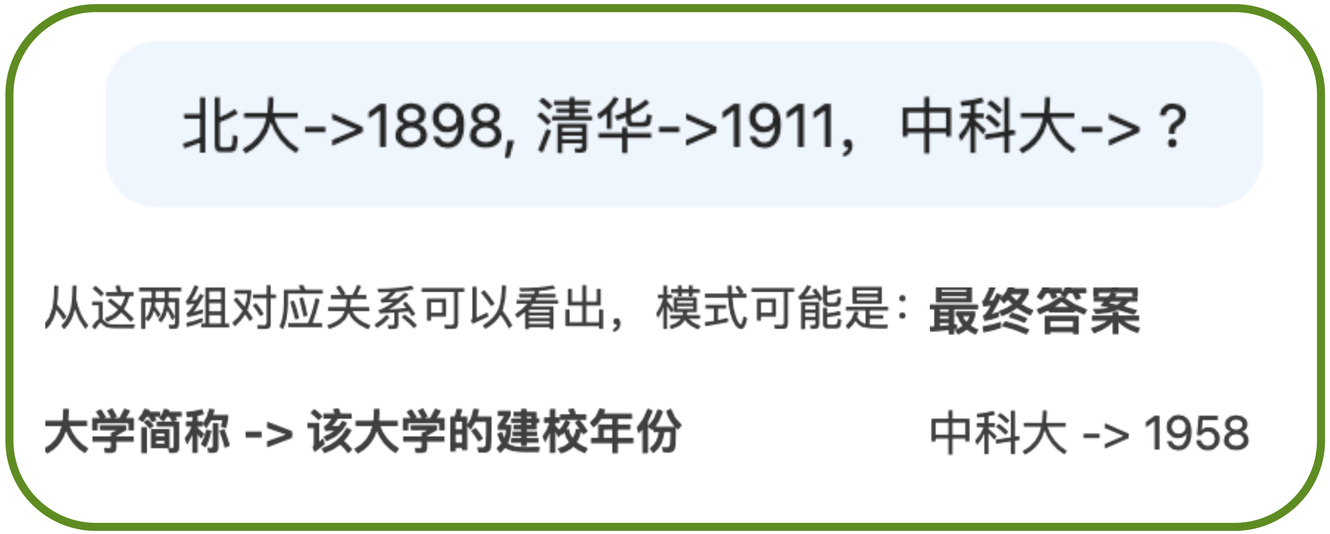

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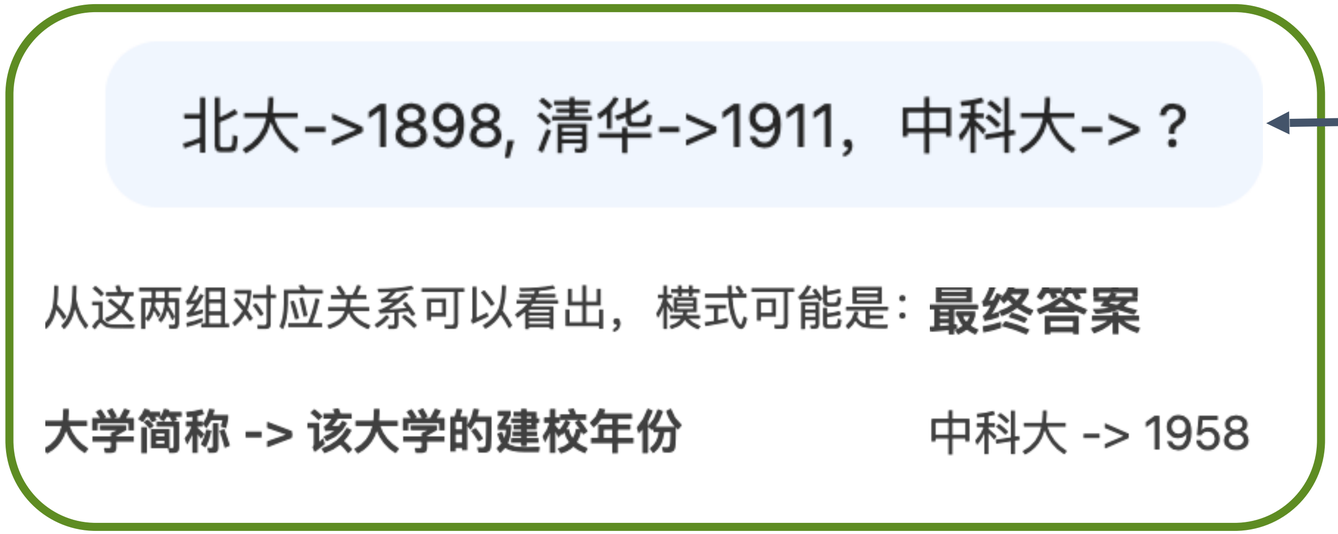

$$\{(X_i, Y_i)\}_{i=1}^{n}, X_{n+1}$$

New training set as examples in prompt

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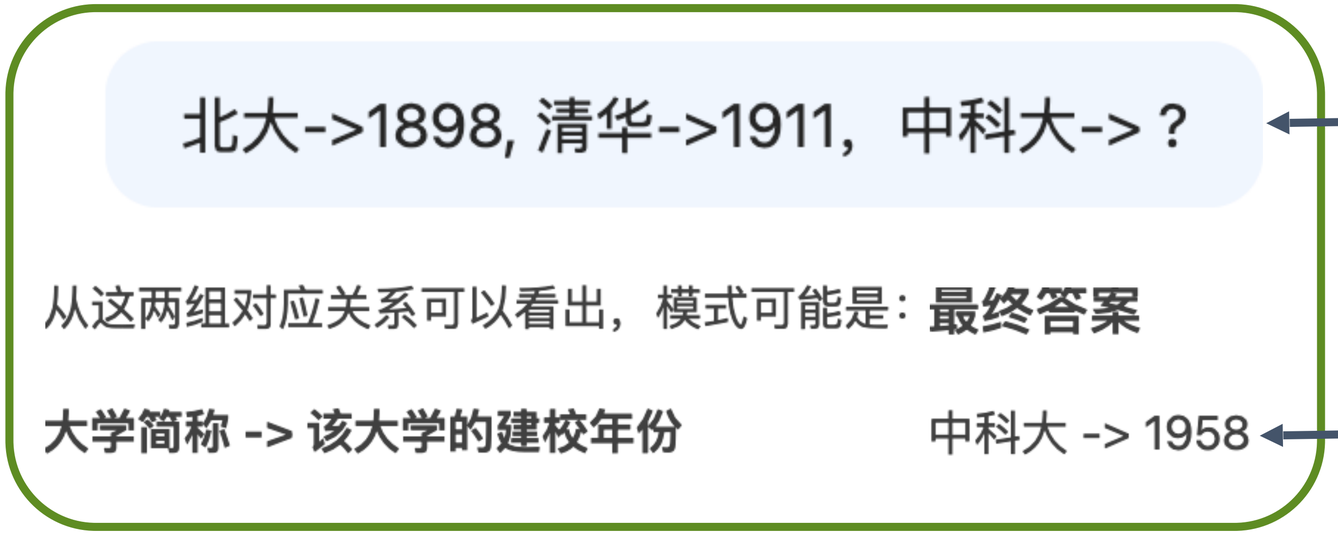

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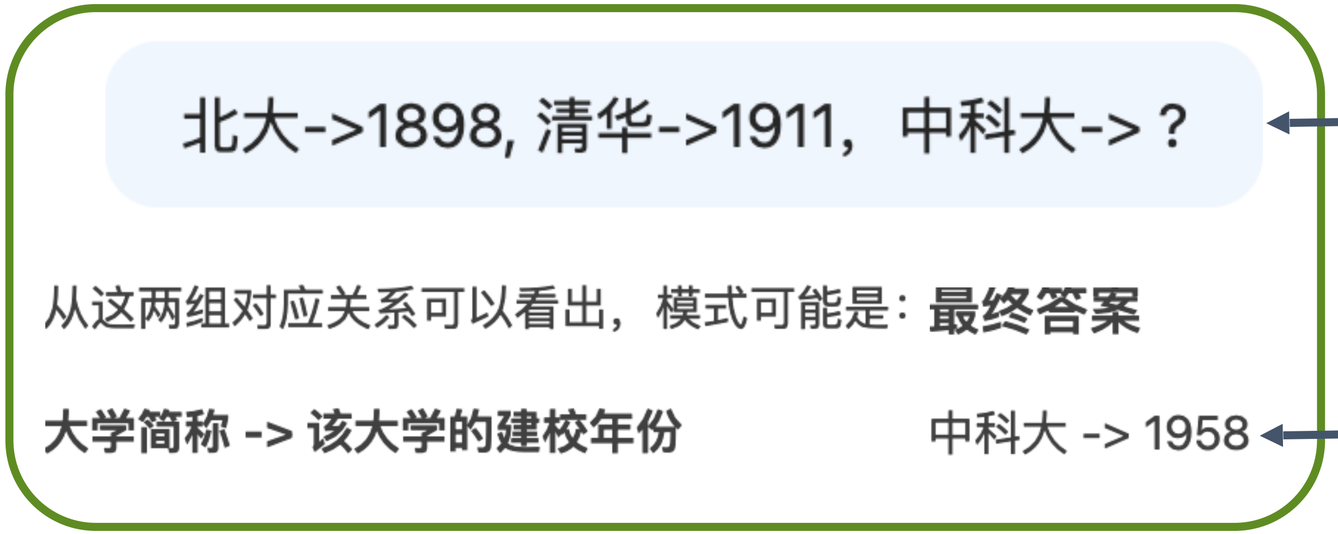

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TabPFN's ICL in statistical language

Amortized Bayesian inference

$$\mathcal{D} = (X_1, Y_1, \ldots, X_n, Y_n) \sim \pi^* \in \Pi$$

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The posterior predictive distribution for Y_{n+1} given $X_{n+1} = x$ is

$$p(y|x, \mathcal{D}) = \int_{\Pi} \pi(y|x) p(\pi|\mathcal{D})\, d\pi$$

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Key innovation

Traditional Bayesian approaches (e.g., MCMC, Variational inference): approximate

$$x \mapsto p(y|x, \mathcal{D})$$

for a **fixed dataset** $\mathcal{D}$

TabPFN: approximate the map **jointly** over x and $\mathcal{D}$

$$(\mathcal{D}, x) \mapsto p(y|x, \mathcal{D})$$

No per-dataset training is required

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Prior fitted network
1. Specifically designed transformer (7M parameters)
2. Trained purely on synthetic datasets (130M datasets)

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Case studies

1 **Semi-supervised parameter estimation**

2 **Heterogeneous treatment effects estimation**

3 **Prediction under covariate shift**

Case studies

We compare with SOTA (recently published in top statistics journal) using their experimental setting.

1 **Semi-supervised parameter estimation**

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Semi-supervised learning

Problem & motivation

Labeled data is limited; unlabeled data is plentiful

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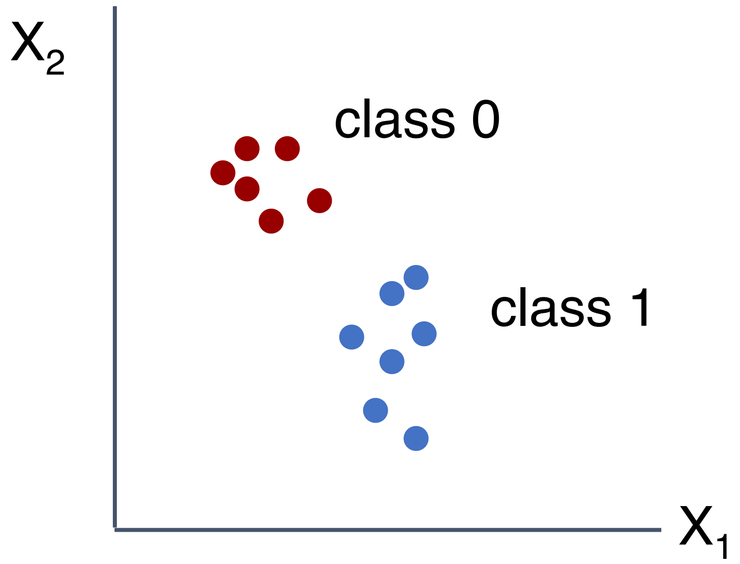

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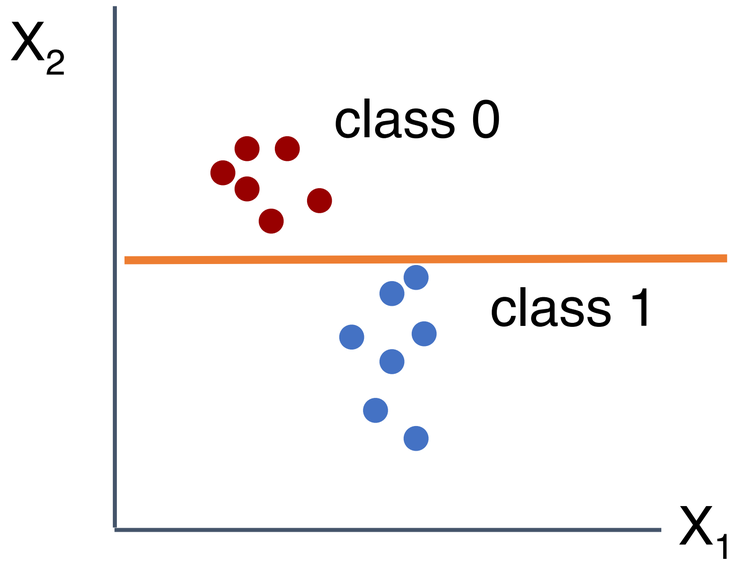

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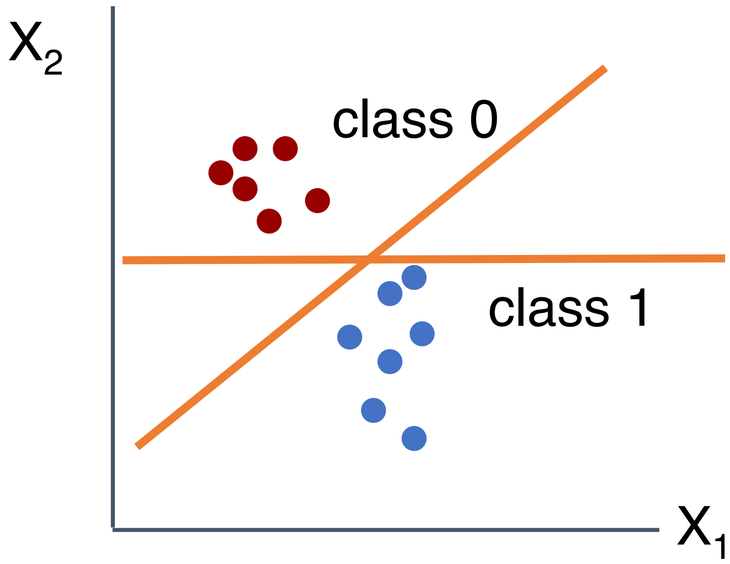

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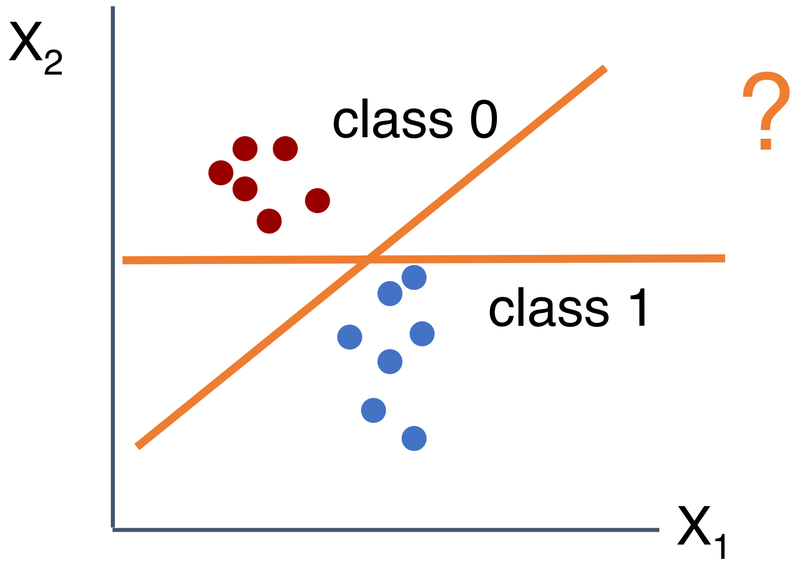

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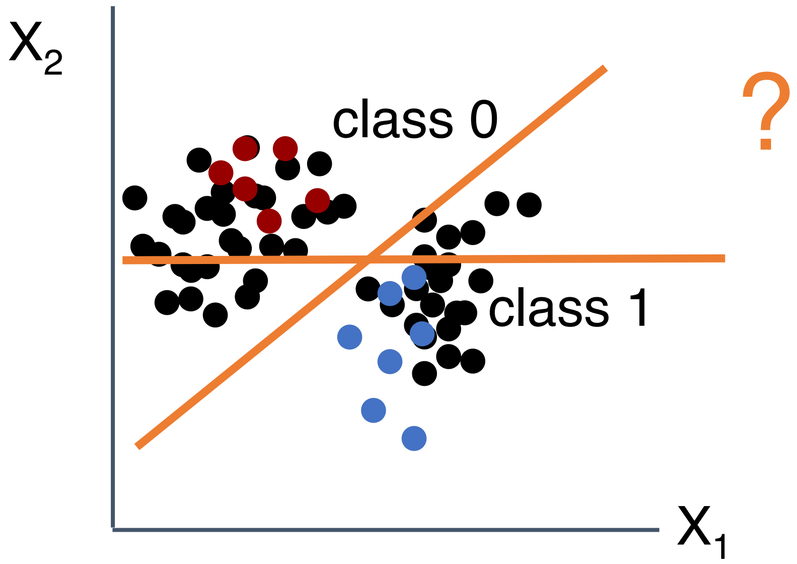

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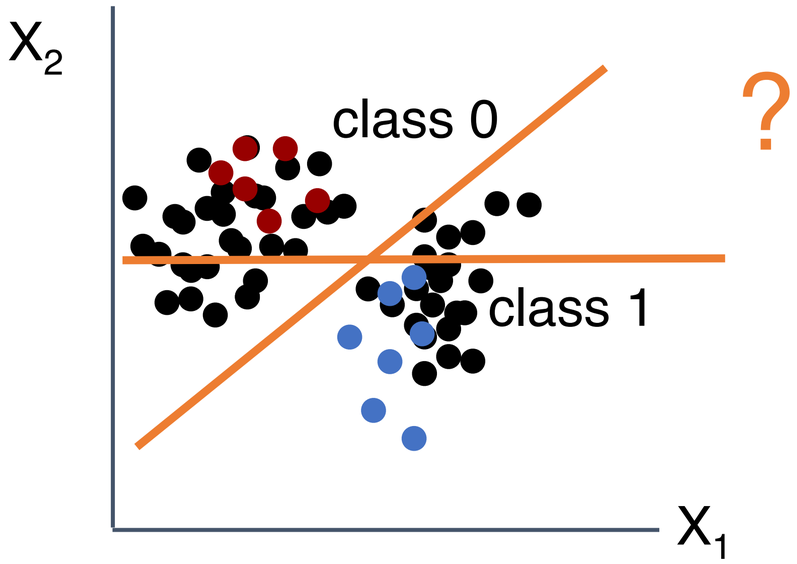

?

n labeled samples $\mathcal{D}_L = \{(X_i, Y_i)\}_{i=1}^{n}$

m unlabeled samples $\mathcal{D}_U = \{X_i\}_{i=n+1}^{n+m}$

$$m \gg n$$

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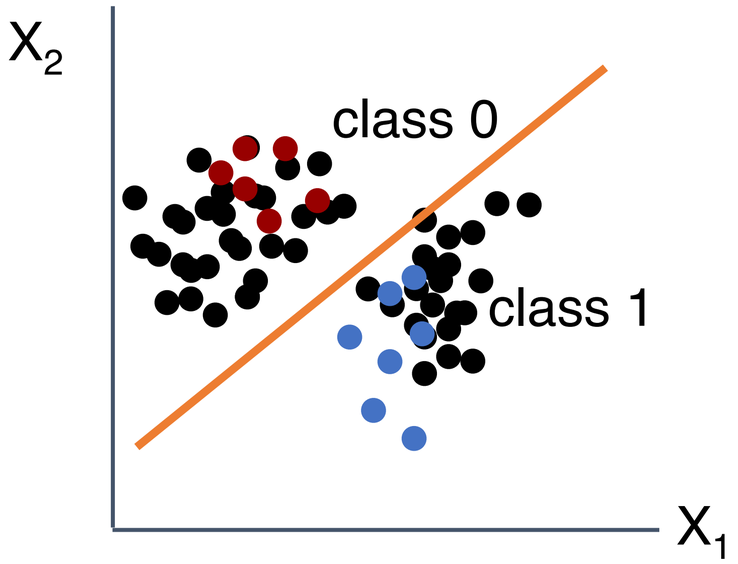

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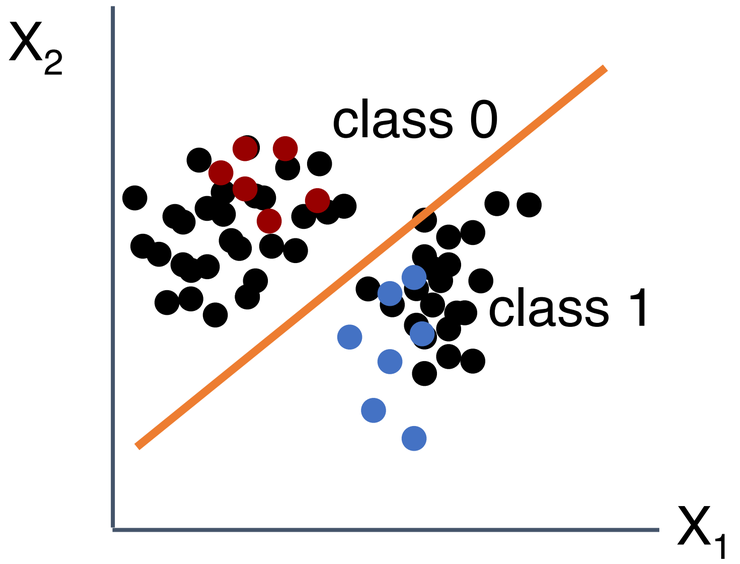

True parameter

$$\theta^* = \text{argmin}_{\theta \in \Theta} \mathbb{E}_{P_{X,Y}} \{ l(\theta; X, Y) \}$$

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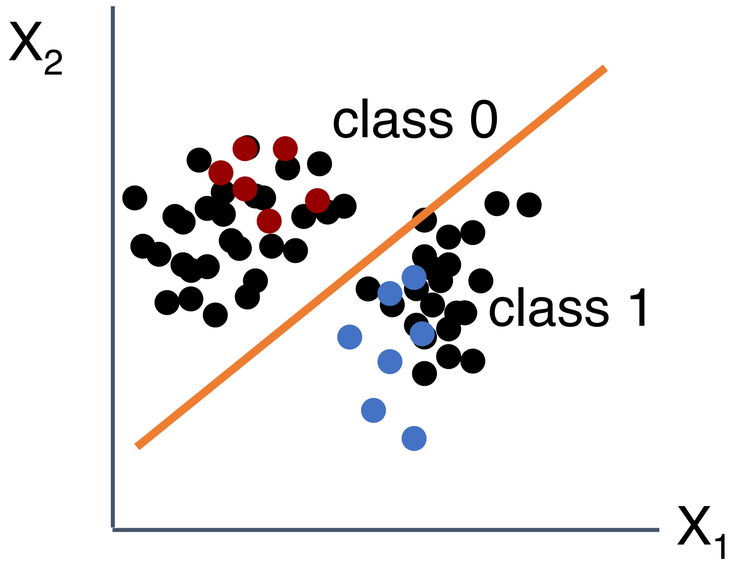

True parameter

$$\theta^* = \text{argmin}_{\theta \in \Theta} \mathbb{E}_{P_{X,Y}} \{ l(\theta; X, Y) \}$$

true distribution of the data

n labeled samples $\mathcal{D}_L = \{(X_i, Y_i)\}_{i=1}^{n}$

m unlabeled samples $\mathcal{D}_U = \{X_i\}_{i=n+1}^{n+m}$

$$m \gg n$$

Semi-supervised learning

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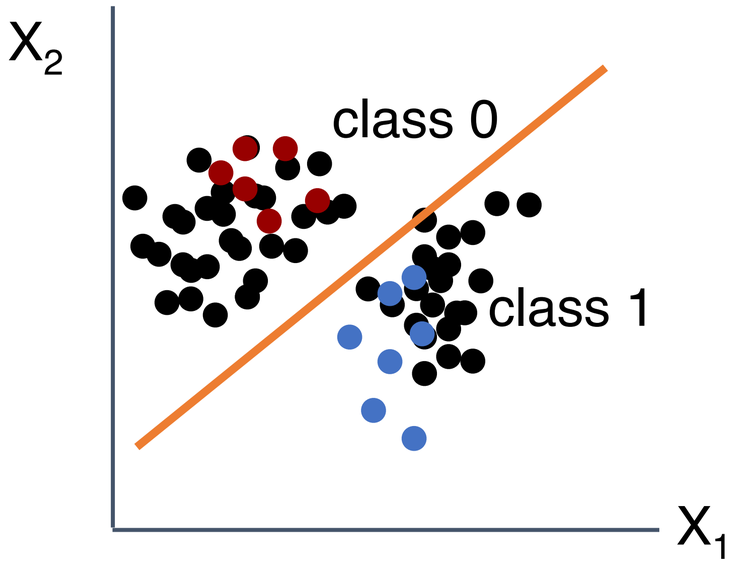

True parameter

self-specified loss function

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Semi-supervised learning

Methods

Semi-supervised learning

Methods

- **SLZ (Song, Lin and Zhou. 2023 JASA) SOTA**

Semi-supervised learning

Methods

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- **Empirical risk minimizer (ERM)**

$$\hat{\theta}_{\mathrm{ERM}}(\mathcal{D}) = \arg\min_{\theta} \sum_{(X,Y)\in\mathcal{D}} l(\theta; X, Y)$$

Semi-supervised learning

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1. Use TabPFN to impute labels: $\hat{\mathcal{D}}_L = \{(X_i, \hat{Y}_i)\}_{i=1}^{n}$ $\hat{\mathcal{D}}_U = \{(X_i, \hat{Y}_i)\}_{i=n+1}^{n+m}$

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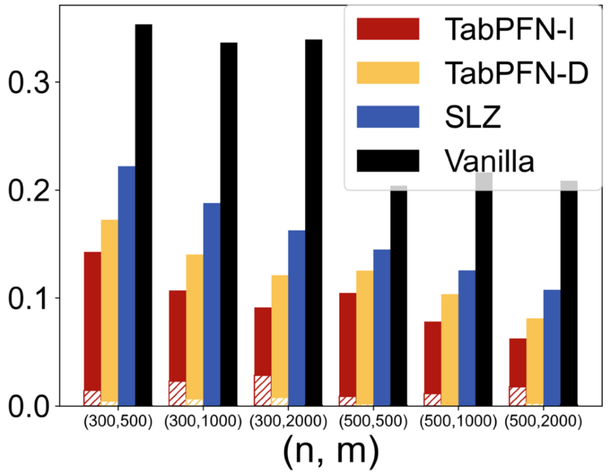
2. **TabPFN-I:** $\hat{\theta}_{\mathrm{ERM}}(\hat{\mathcal{D}}_L \cup \hat{\mathcal{D}}_U)$
3. **TabPFN-D(Angelopoulos et al. 2023 Science):**
   - estimate the imputation bias by $\Delta = \hat{\theta}_{\mathrm{ERM}}(\hat{\mathcal{D}}_L) - \hat{\theta}_{\mathrm{ERM}}(\mathcal{D}_L)$
   - return the estimator $\hat{\theta}_{\mathrm{ERM}}(\hat{\mathcal{D}}_L \cup \hat{\mathcal{D}}_U) - \Delta$

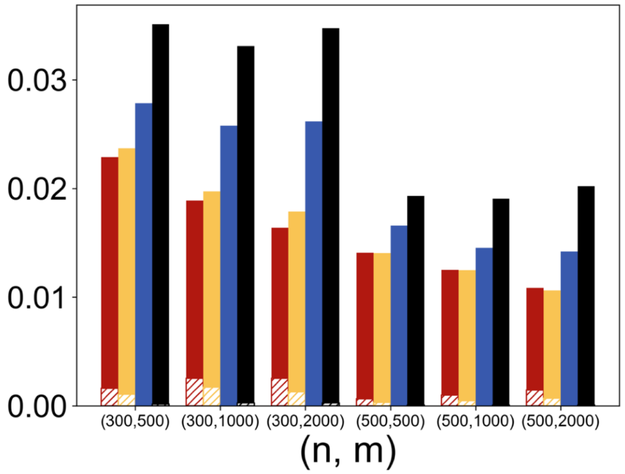
Semi-supervised learning

Empirical results

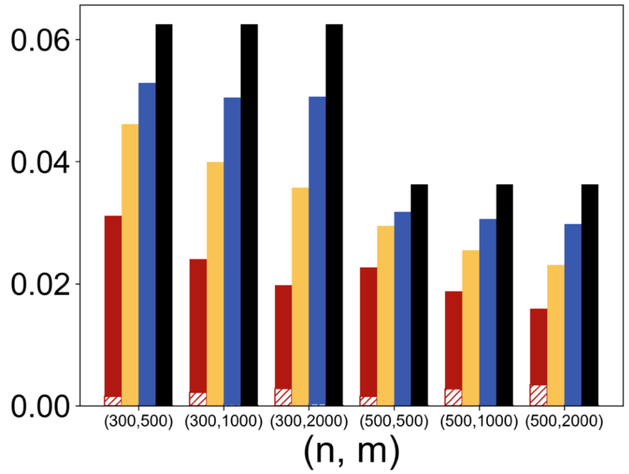
Variance Bias^2



Linear regression



Logistic regression



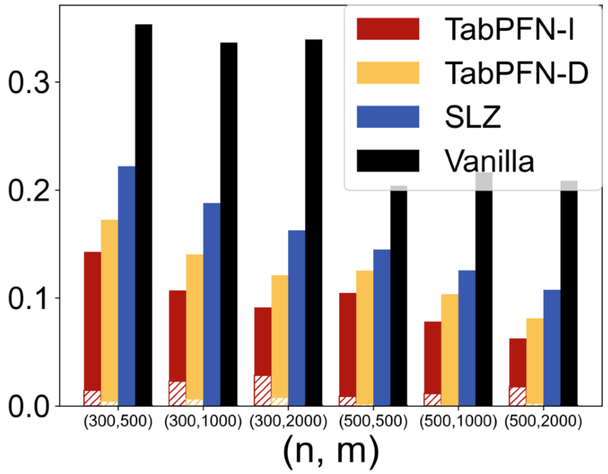
Quantile regression

Semi-supervised learning

Empirical results

TabPFN beats SOTA in estimating regression coefficients when model is misspecified

Variance Bias^2



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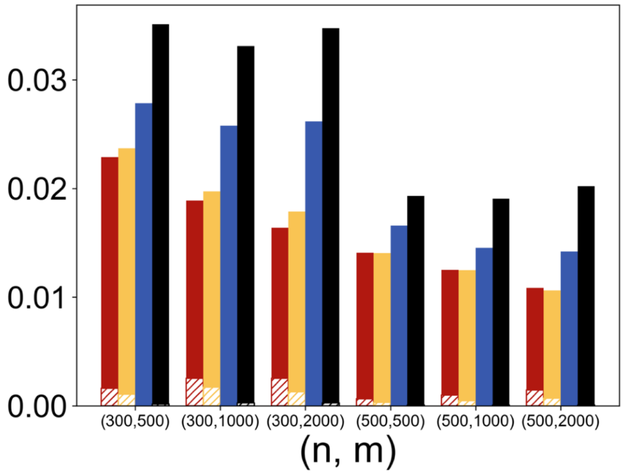

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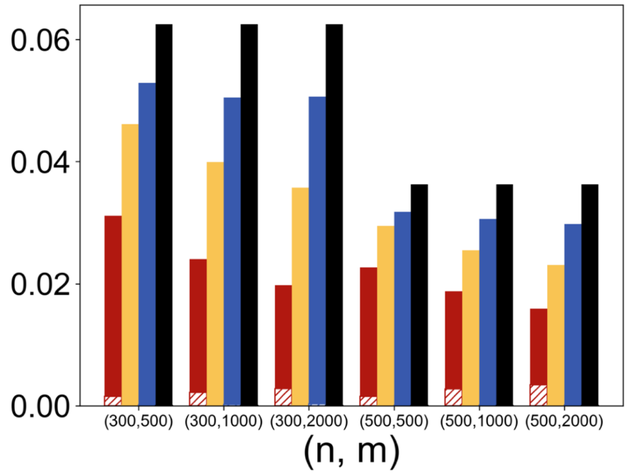

Quantile regression

Heterogeneous treatment effects estimation

Problem & motivation

Heterogeneous treatment effects estimation

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Heterogeneous treatment effects (HTE): how different groups of individuals benefit differentially from the same treatment

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Potential outcome framework:

- Binary treatment: $T_i \in \{0, 1\}$
- Potential outcomes: $Y_i(0), Y_i(1)$ (control/treatment), $Y_i^{\text{obs}} = Y_i(T_i)$
- Average treatment effect (ATE): $\tau = \mathbb{E}\{Y(1) - Y(0)\}$
- Conditional average treatment effect (CATE):

$$\tau(x) = \mathbb{E}\{Y(1) - Y(0) \mid X = x\}$$

Heterogeneous treatment effects estimation

Problem & motivation

Heterogeneous treatment effects (HTE): how different groups of individuals benefit differentially from the same treatment

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Goal: Estimate this function

CATE estimators

Two “nuisance” parameters:

- Response functions: $\mu_j(x) = \mathbb{E}\{Y(j) \mid X = x\}, \quad j = 0, 1$
- Propensity score: $e(x) = \mathbb{P}\{T = 1 \mid X = x\}$

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$$\tau(x) = \mu_1(x) - \mu_0(x)$$

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Idea: **Metalearner framework (Kunzel et al., 2019)**

- Step 1: Estimate $e(x)$ and/or $\mu_j(x)$ using regression and classification algorithms — **base learners**
- Step 2: Combine (in some way) to get estimate for $\tau(x)$ — **meta-learners**

CATE estimators

S-learner

1. Form an estimator $\hat{\mu}(t, x)$ for the function
$$(t, x) \mapsto \mu_t(x)$$
by jointly regressing Y_i^{obs} on T_i and X_i
1. S-learner is

$$\hat{\tau}_S(x) = \hat{\mu}(1, x) - \hat{\mu}(0, x)$$

DR-learner SOTA

1. Form estimates $\hat{\mu}_j(x)$ for $\mu_j(x)$, and $\hat{e}(x)$ for propensity score
2. Compute doubly robust pseudo-outcomes $\tilde{Y}_i$
3. Estimate CATE by regressing $\tilde{Y}_i$ on X_i

$$\tilde{Y}_i = \frac{T_i(Y_i - \hat{\mu}_1(X_i))}{\hat{e}(X_i)} - \frac{(1-T_i)(Y_i - \hat{\mu}_0(X_i))}{1-\hat{e}(X_i)} + \hat{\mu}_1(X_i) - \hat{\mu}_0(X_i)$$

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Current emphasis:

- Choice of meta-learner more important than base learner
- DR-learner achieves optimal asymptotic rates (under smoothness assumptions)

CATE estimation

Experimental design

Followed Foster and Syrgkanis (2023 AOS) setting

$$T_i \sim \text{Bern}(e(X_i)), \quad X_i \sim U([-0.5, 0.5]^6)$$

$$Y_i \sim \tau(X_i)(T_i - 1/2) + b(X_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

Setup A: complicated $e(x)$ and $b(x)$, but a relatively simple $\tau(x)$
Setup B: large $b(x)$ resulting in substantial confounding, discontinuous $\tau(x)$

Base-learner: estimators for the regression functions (Auto-ML or TabPFN)

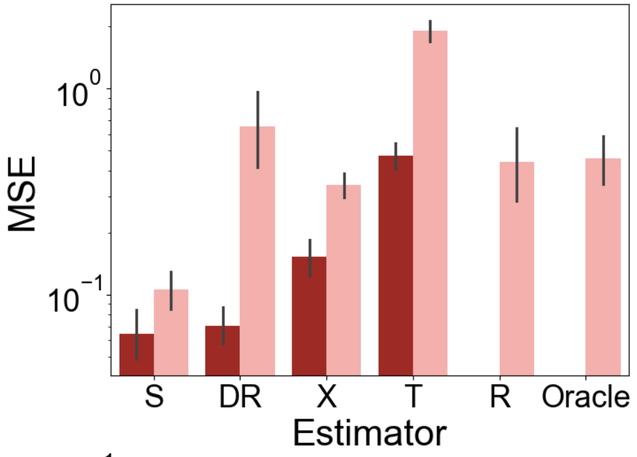
CATE estimation

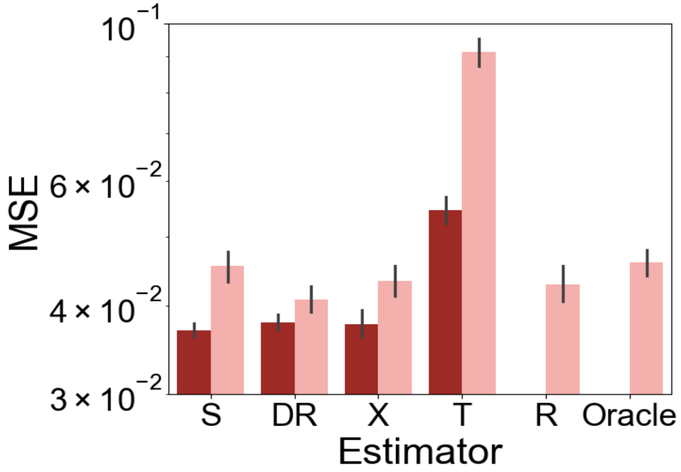
Results

small-sample high variance

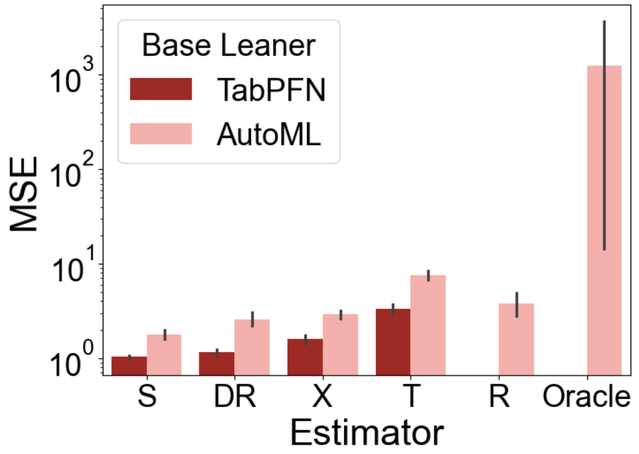
large-sample low variance

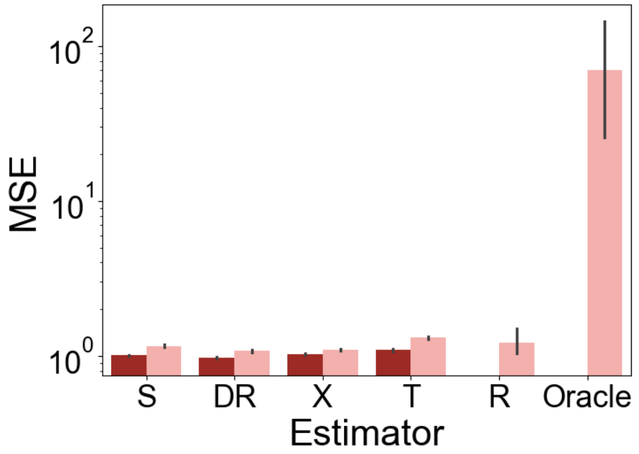
Setup A





Setup B





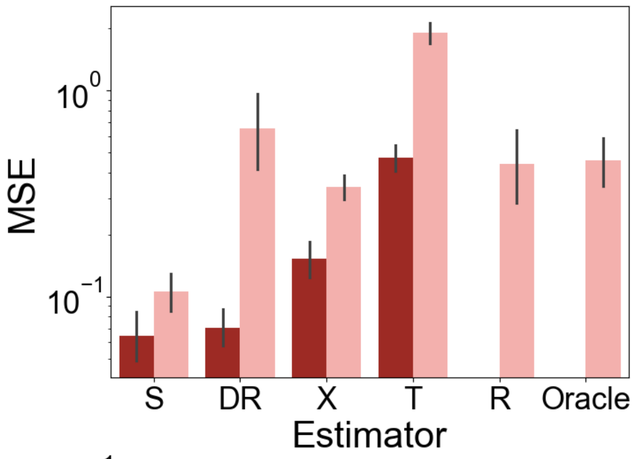
CATE estimation

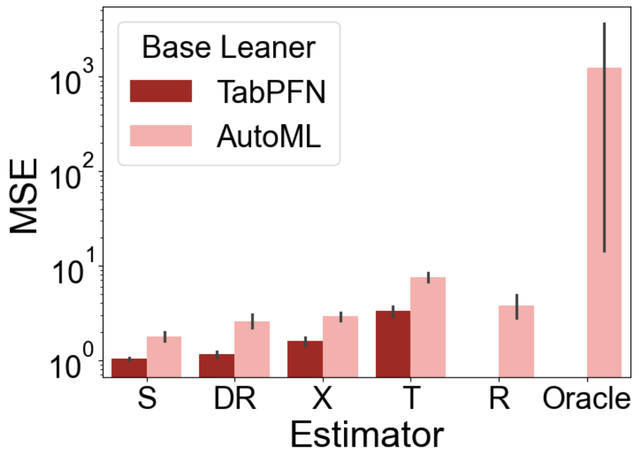
Results

TabPFN > AutoML; S-Learner (TabPFN) wins without double robustness; base learner choice is important

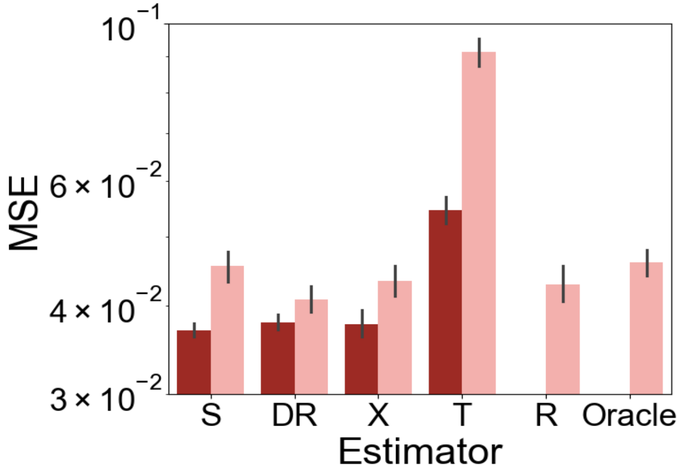
Setup A | **Setup B**

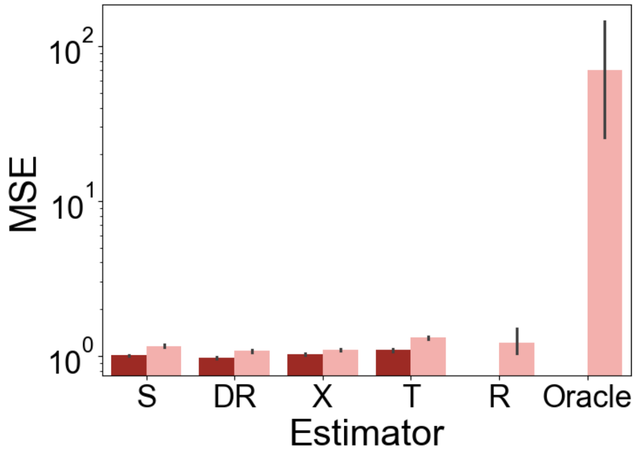
small-sample high variance





large-sample low variance





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TabPFN adapts flexibly to various functional structures and can leverage parametric structures, even outperforming specialized methods.

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TabPFN adapts flexibly to various functional structures and can leverage parametric structures, even outperforming specialized methods.

1. **Flexible but distinct from GPs:** Like Gaussian processes, TabPFN adapts to any function in low dimensions, but differs in extrapolation, ease of step-function fitting, and handling rapid variations.

1. **Sparsity-dependent performance:** Outperforms LASSO in high-sparsity/low-SNR regimes but lags in dense linear regression (≥20 features).

1. **Robust & efficient classifier:** Robust to label noise and also efficient..

Paper link

Summary

1. TabPFN achieves significantly better estimation accuracy than the comparator methods.

2. TabPFN is NOT a perfect model.

3. The ideas of “in-context learning” and “foundation model” have the potential to supersede existing modeling approaches on a wide range of statistical tasks

4. **We should engage with this opportunity!**