# Comparing Modern Machine Learning Methods for Predicting Individual Treatment Effect

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# Motivation

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- **not all participants will react equally to an intervention**
- Characterizing this **heterogeneity in intervention effects** is key to improving patients outcomes.

# Objective

In order **to estimate Individual Treatment Effects**.

To compare state-of-the-art **Statistical models and Machine Learning algorithms**.

# The predicted individual treatment effects **(PITE)** framework

- **PITE is a method to estimate individual treatment effects**.

**challenge**

PITE is unobserved

# The predicted individual treatment effects **(PITE)** framework

- PITE consists of the difference between **experimental(E) and control (C) prediction** for each individual [Jaki et al., 2024].

$$\text{PITE}_i = f_E(\boldsymbol{X}_i) - f_C(\boldsymbol{X}_i), \qquad f(\cdot) \text{ is a predictor}$$

**?**

Which method is the best to estimate PITE

# Can any approach for prediction be applied?

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- population heterogeneity,
- complex structures (linear/non-linear)
- and high-dimensionality [Lamont et al., 2016].

# Can any approach for prediction be applied?

**important!**

- The best method to estimate the PITE is not **necessarily** the best fit model.
- An essential part is **to delineate this heterogeneity** based on the baseline covariates (features).

# Regressions approaches applied

# Metrics

- The risk (Expected Prediction Squared Error)

$$\frac{1}{n}\sum_{i=1}^{i=n}(\text{tPITE}_i - \text{PITE}_i)^2 \times 100$$

- Sensitivity (Detect PITE direction)

$$\text{Same Direction}_i = \begin{cases} 1 & \text{if } \text{tPITE}_i \times \text{PITE}_i > 0 \\ -1 & \text{otherwise} \end{cases}$$

true $\text{tPITE}_i$ and estimated $\text{PITE}_i$.

# Data generation mechanism

Sample size $n = 40, 70, 100, 300, 400, \mathbf{500}, \mathbf{1000}, 1200, 1500$ with allocation ratio 1:1 ($n_C = n_T = n/2$).

$$y = \boldsymbol{X}\beta + t\boldsymbol{Z}\gamma + \epsilon, \quad \epsilon \sim N(0, 1)$$

$t \in (0, 1) \Rightarrow$ benefit $\boldsymbol{Z}\gamma$

Split the population 70% for training and 30% for validation.

- $\boldsymbol{Z}$ Normal, Linear, High correlations **(up to 0.5)**

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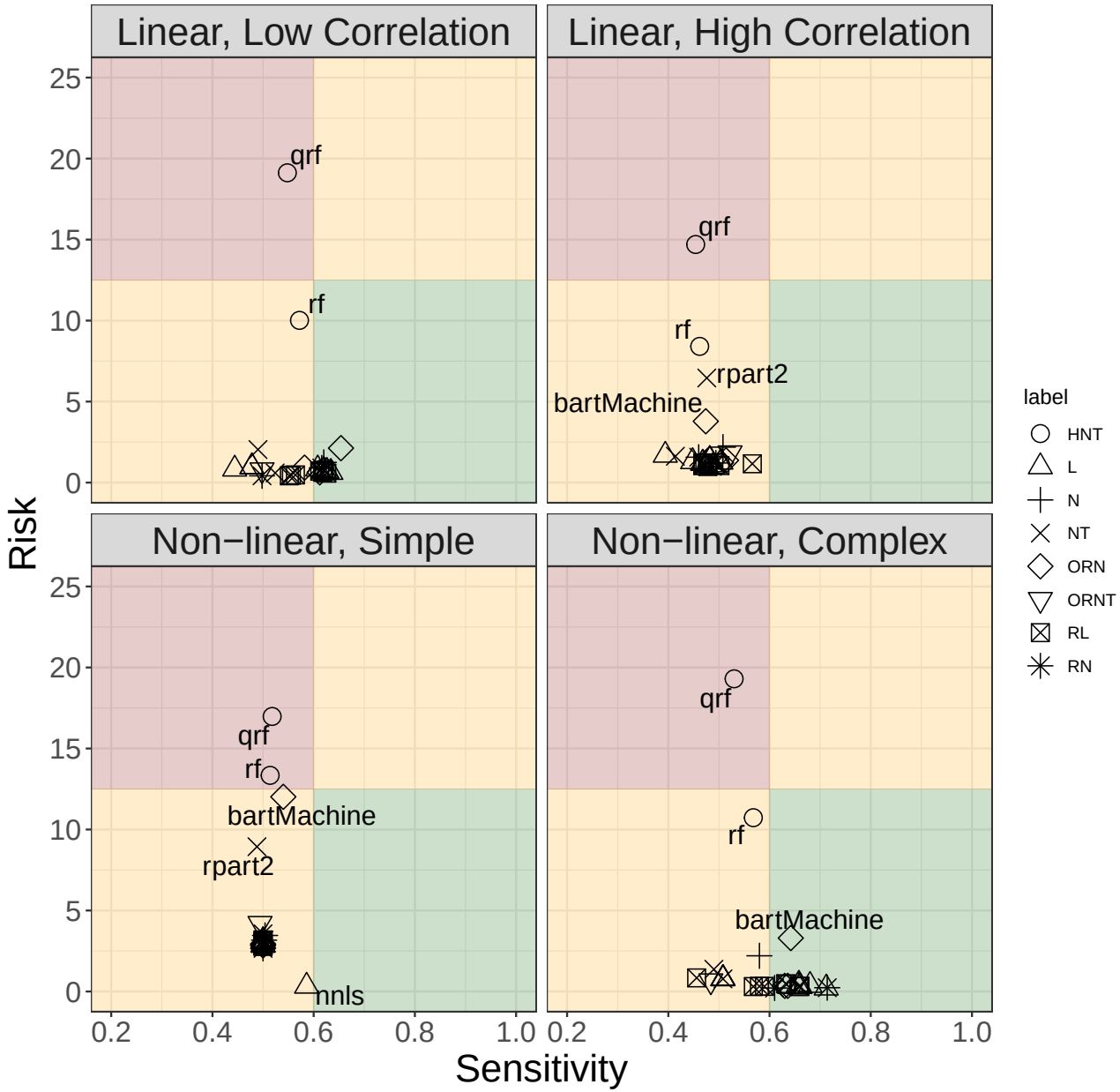
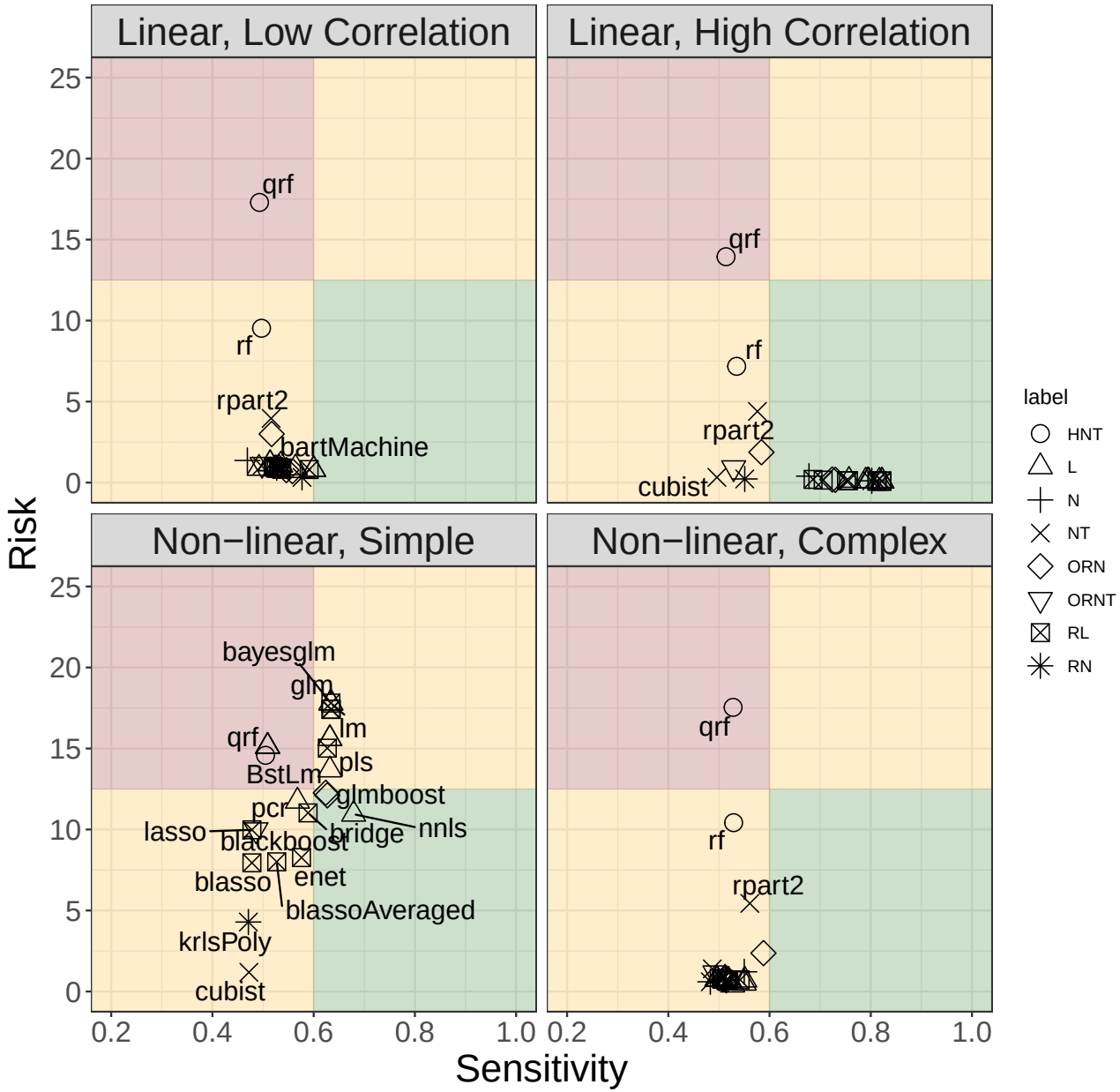
- $\boldsymbol{Z} \sim U[0.1, 0.5]$, Non-linear. Benefit: $\frac{\log(Z_1)\gamma_0}{Z_1{}^{\gamma_2} - \gamma_3\sqrt{Z_2+2}}$

# Highlight based on risk and sensitivity $n = 500$

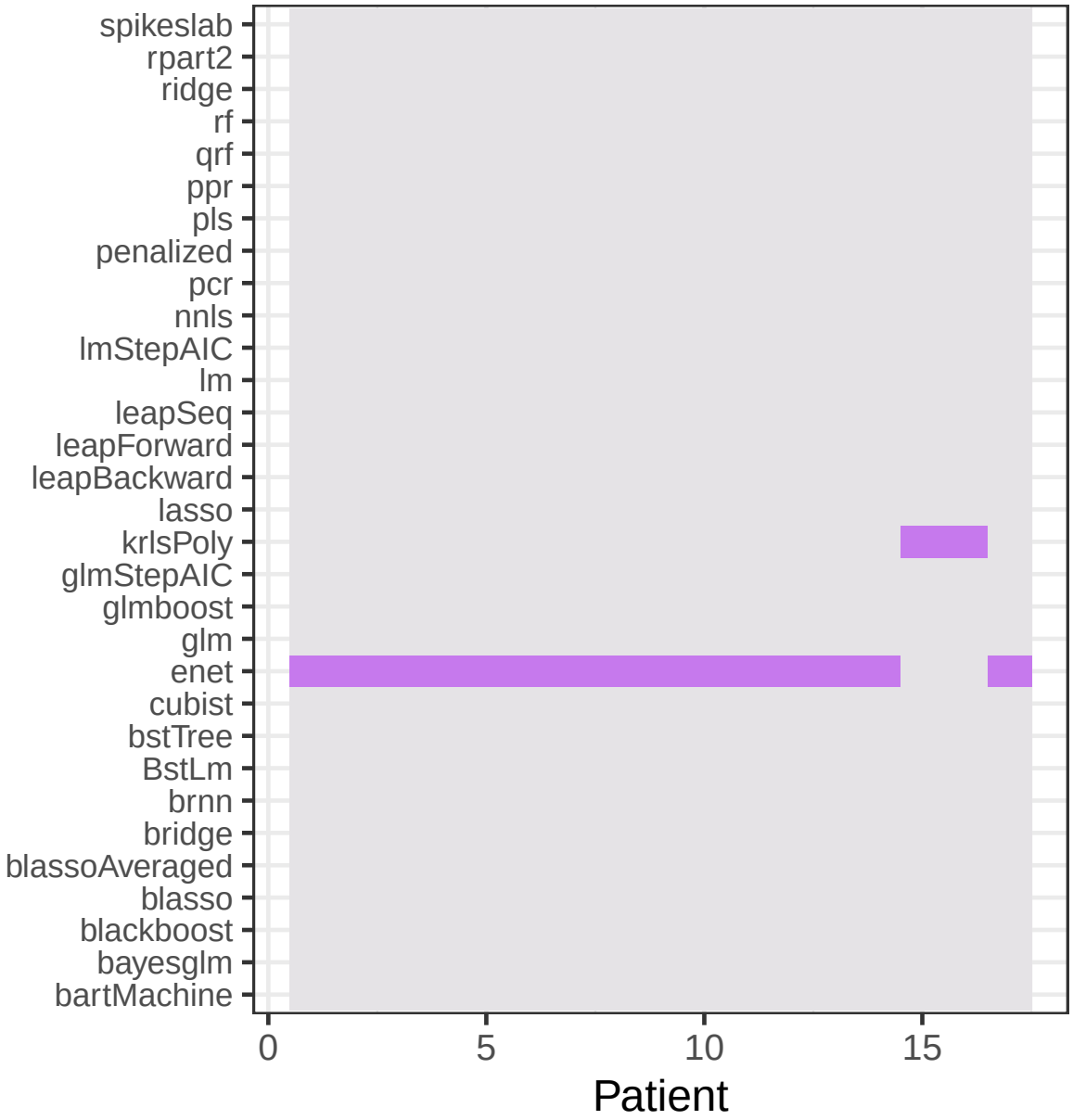


# Highlight based on risk and sensitivity $n = 1000$



# Difficult cases Non-lin Complex $n = 500$

only **one model** captures the PITE direction



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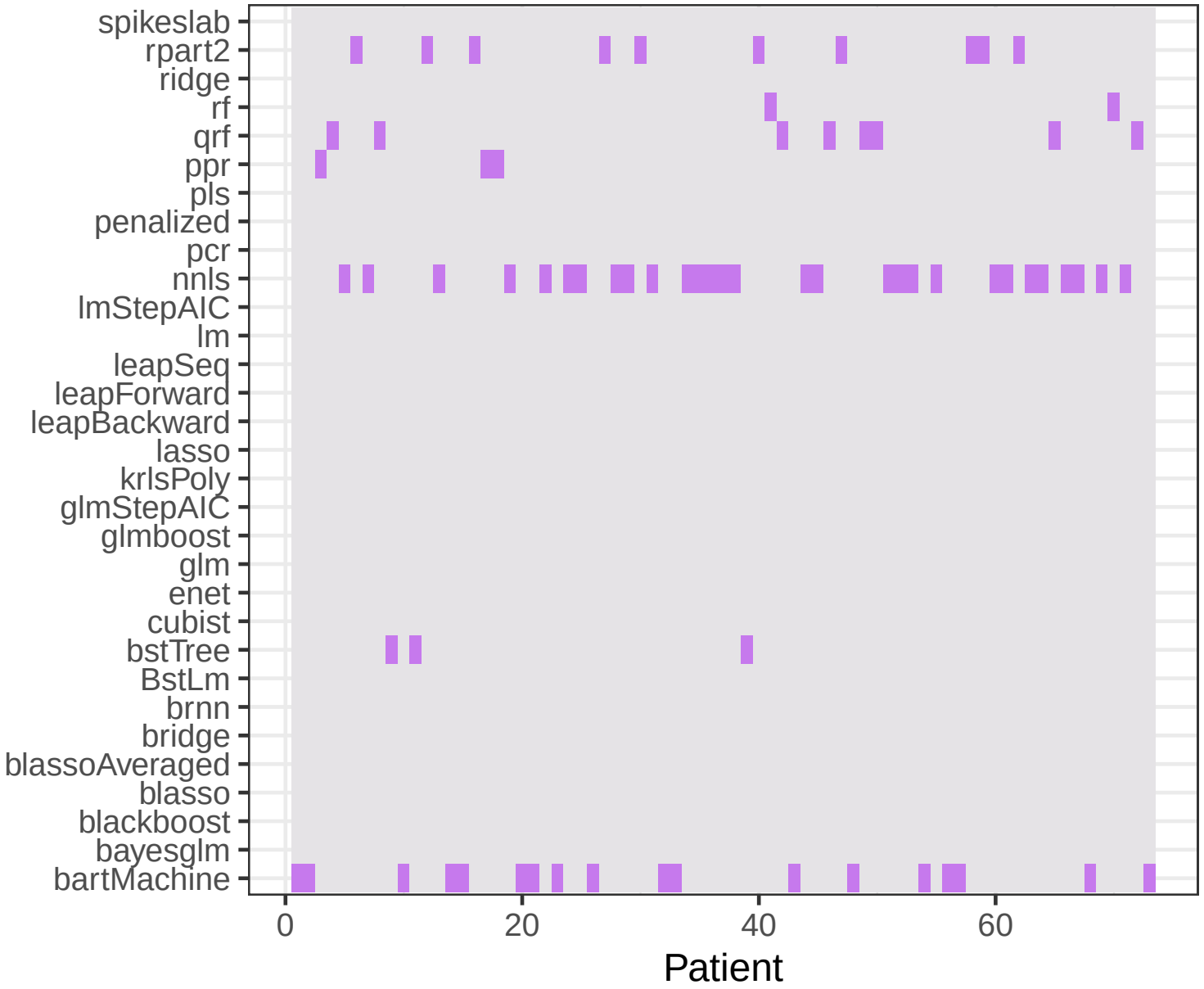

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- An analyst should know what characteristics their dataset presents.
- For each situation sensitivity varies little for different methods.
- Risk is more variable.
- Some methods benefit more from smaller sample size.
- Leave complex methods for large sample size.

# References I


Thomas Jaki, Chi Chang, Alena Kuhlemeier, and M. Lee Van Horn. Predicting individual treatment effects: Challenges and opportunities for machine learning and artificial intelligence. *KI - Künstliche Intelligenz*, January 2024. ISSN 1610-1987. doi: 10.1007/s13218-023-00827-4. URL http://dx.doi.org/10.1007/s13218-023-00827-4.

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