Conformal Meta-learners for Predictive Inference of Individual Treatment Effects

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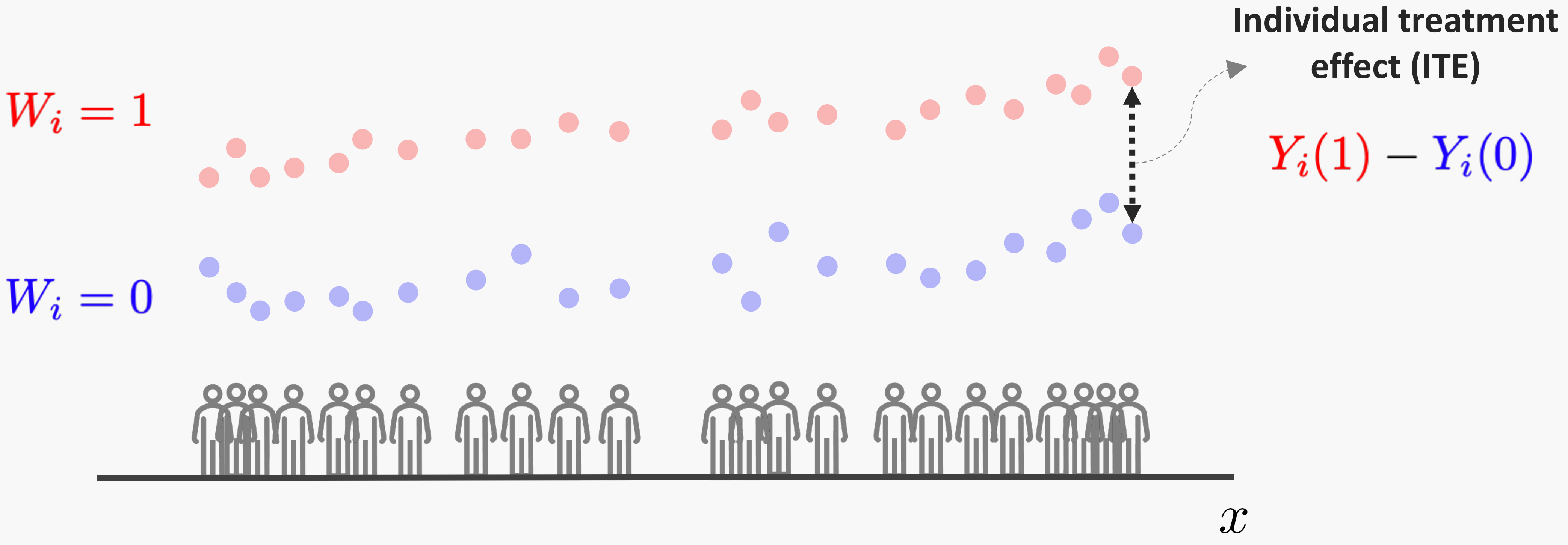
Setup: Potential Outcomes Framework

(Neyman 1923; D. Rubin 1974)

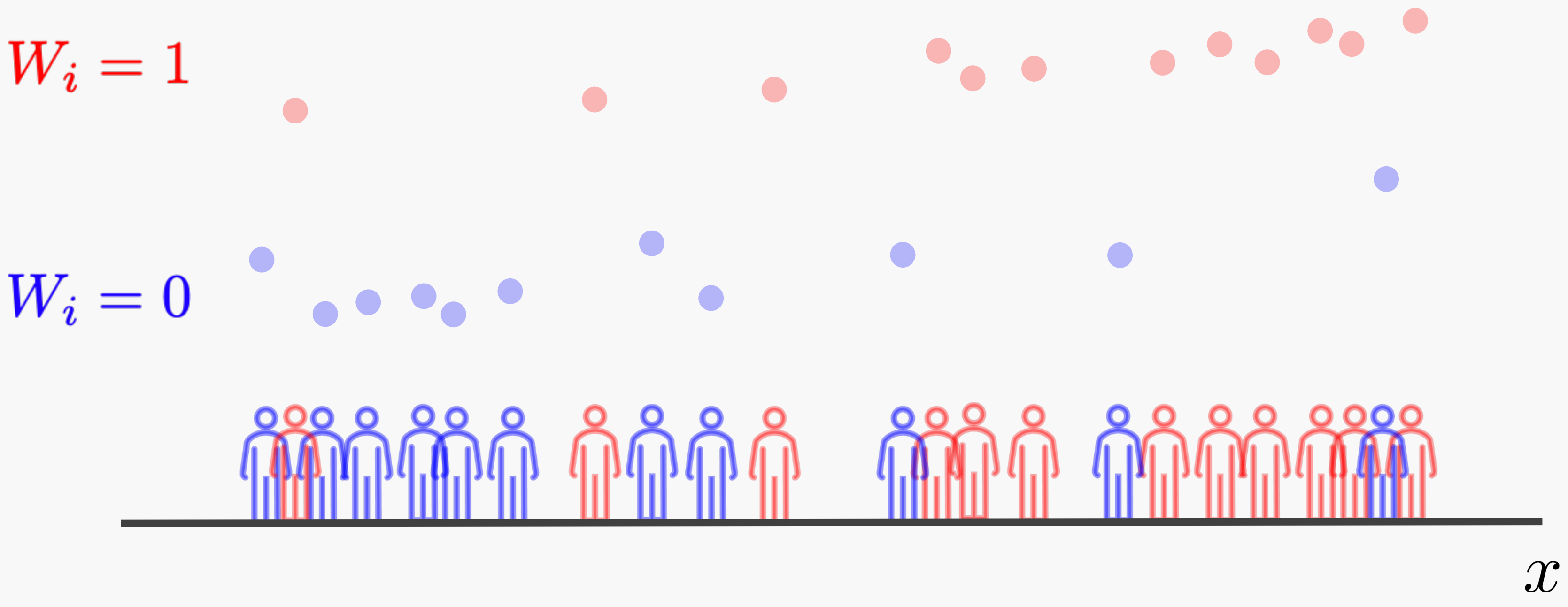
- Binary treatment $W_i \in \{0,1\}$ → two potential outcomes: $Y_i(1)$ and $Y_i(0)$



Setup: Potential Outcomes Framework

- **The fundamental problem of causal inference:** Counterfactuals are not observed!

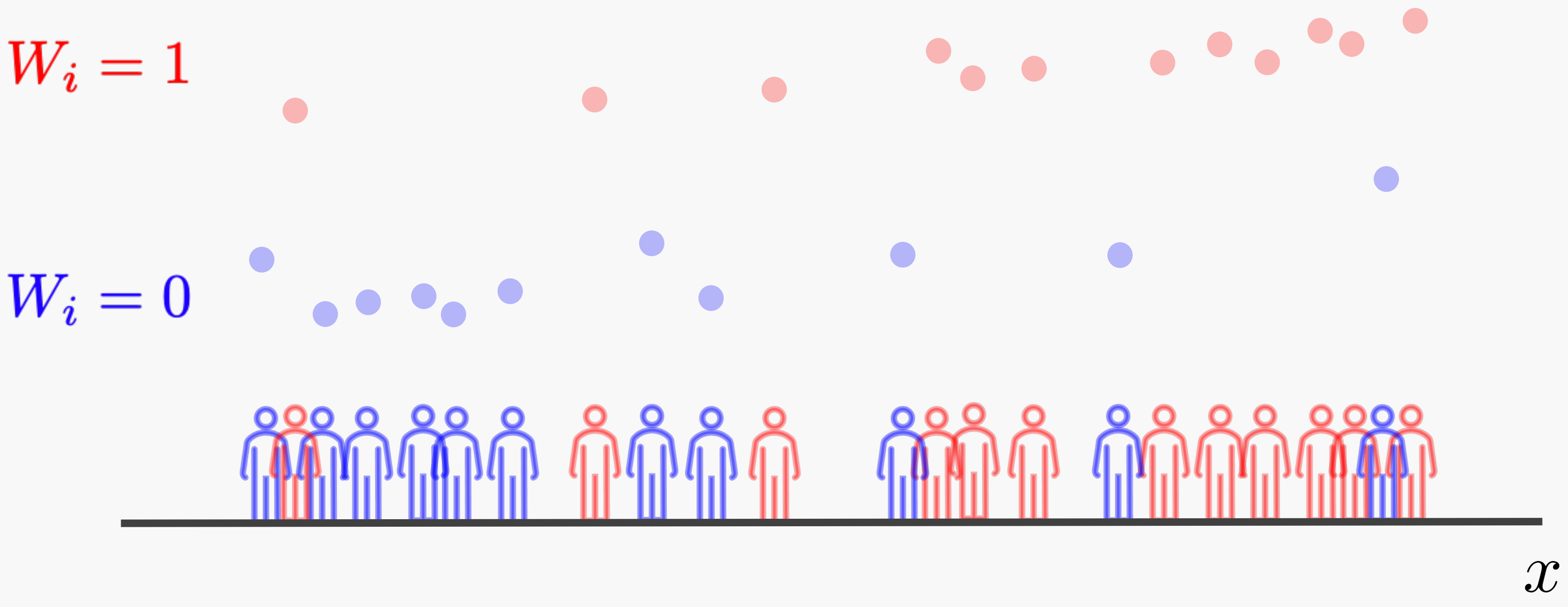
$$Y_i = W_i Y_i(1) + (1 - W_i) Y_i(0)$$



Setup: Potential Outcomes Framework

- **Treatments not randomly assigned:** Propensity score → $\pi(x) = P(W = 1 | X = x)$

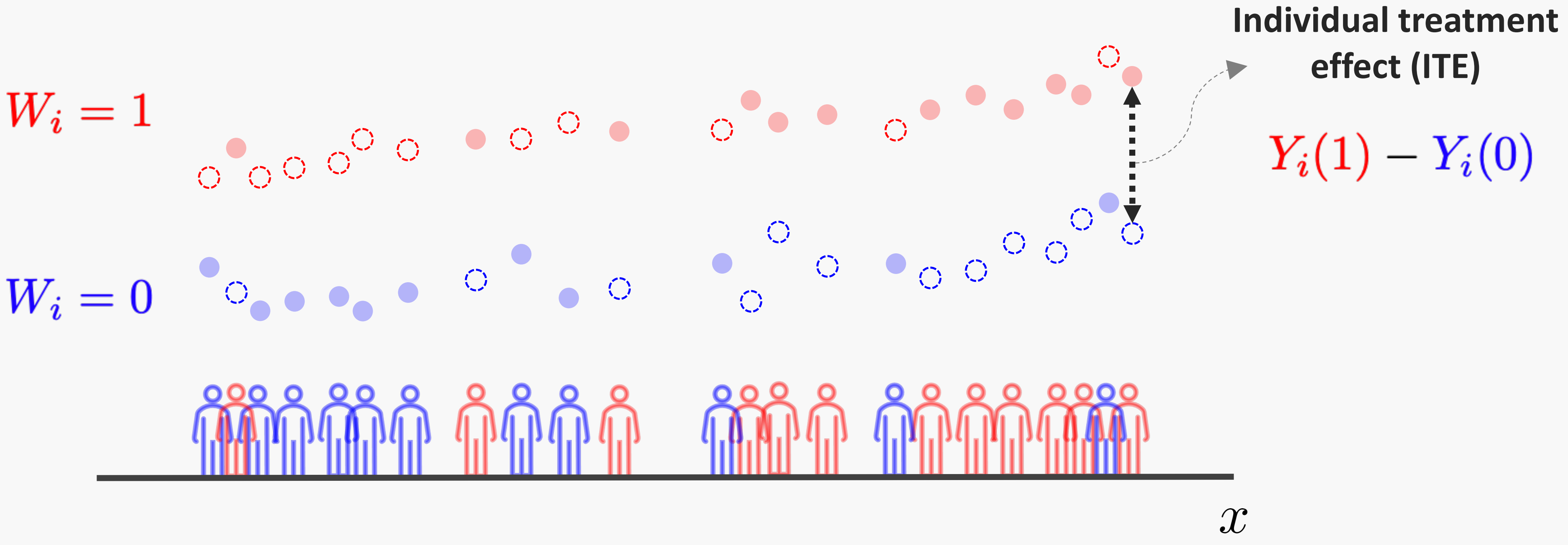
$$Y_i = W_i Y_i(1) + (1 - W_i) Y_i(0)$$



Problem: Valid Predictive Inference on ITEs

- **Predictive Inference:** Construct predictive intervals $\widehat{C}(X_{n+1})$ that cover ITEs

$$P(Y_{n+1}(1) - Y_{n+1}(0) \in \widehat{C}(X_{n+1})) \geq 1 - \alpha$$



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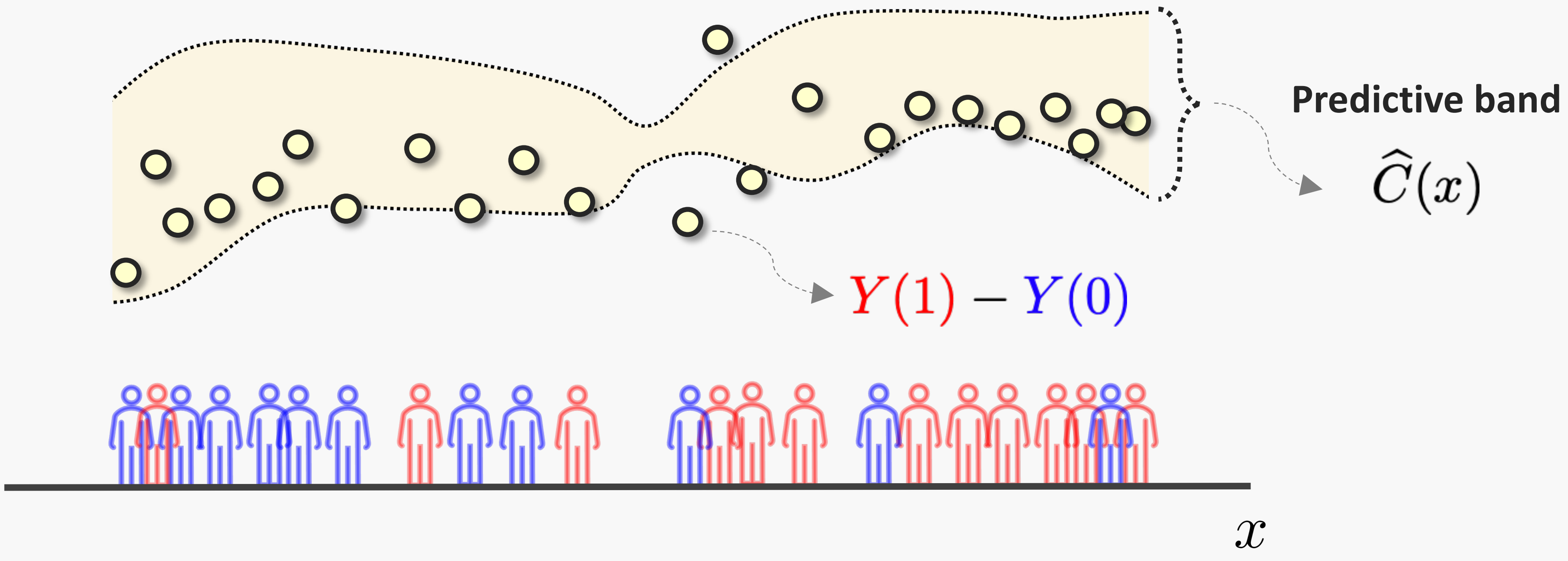
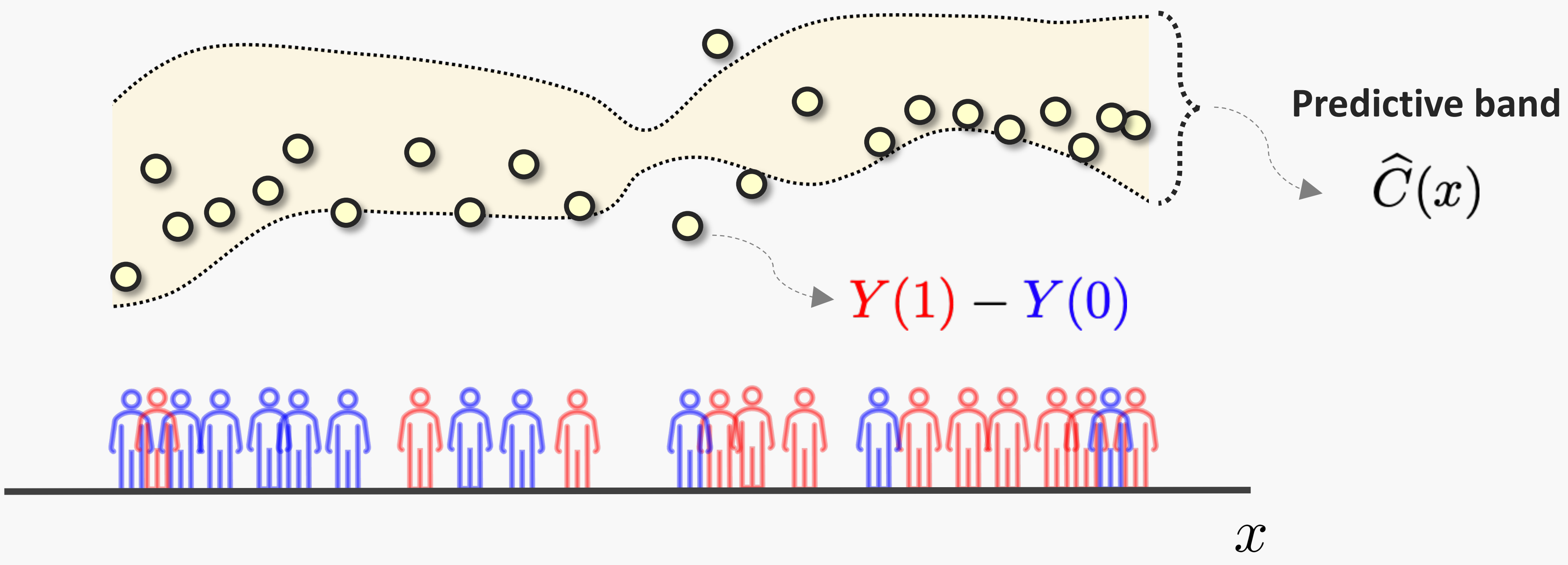


Proposed Method: Conformal Meta-Learners

Concept 1:
Pseudo-outcome Regression

Concept 2:
Conformal Prediction



Concept 1: Pseudo-outcome Regression (Meta-learners)

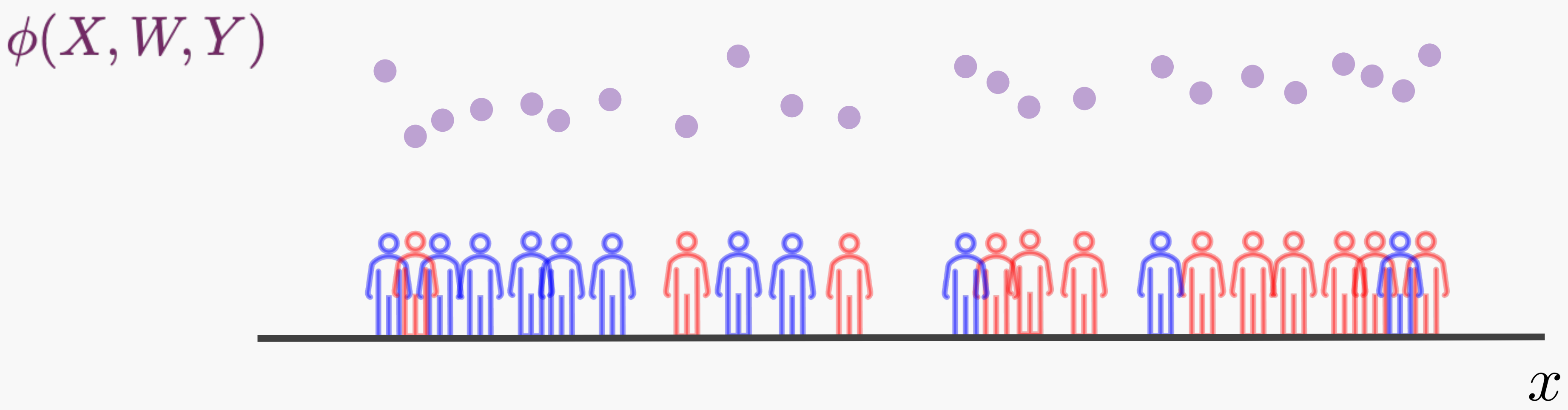
(van der Laan 2006; E. Kennedy 2020 and others)

- **Pseudo-outcomes:** Transformations of (X, W, Y) that preserve conditional effects

$$E[\phi(X, W, Y)|X = x] = E[Y(1) - Y(0)|X = x]$$

Inverse Propensity Weighting

$$\phi_{\text{IPW}} = \frac{W - \pi(X)}{\pi(X)(1 - \pi(X))} Y$$



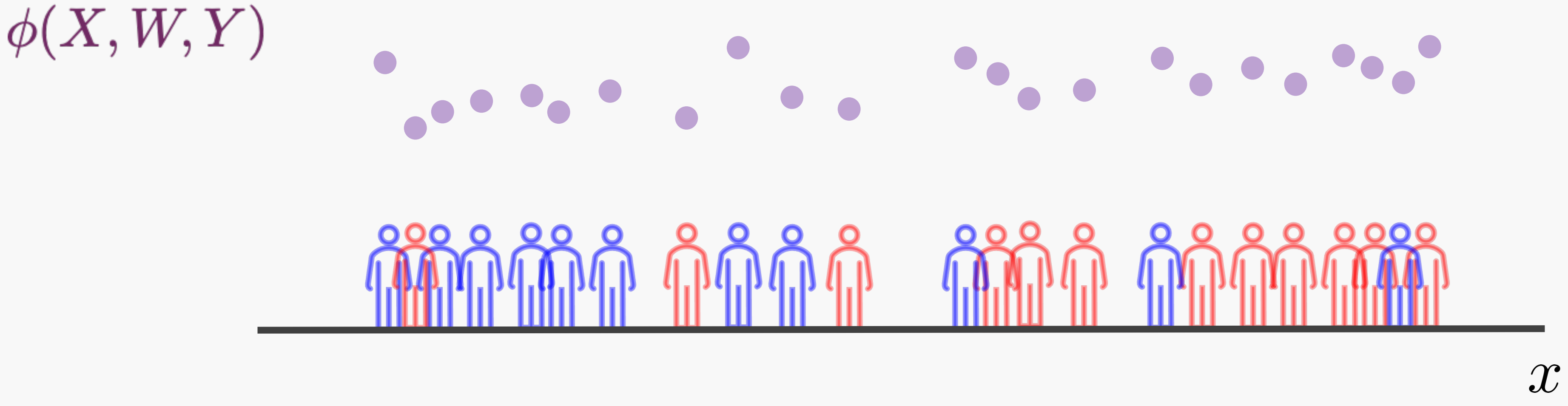
Concept 1: Pseudo-outcome Regression (Meta-learners)

(van der Laan 2006; E. Kennedy 2020 and others)

- **Pseudo-outcomes:** Transformations of (X, W, Y) that preserve conditional effects

$$E[\phi(X, W, Y) | X = x] = E[Y(1) - Y(0) | X = x]$$

$$\tau = E[Y(1) - Y(0)] \rightarrow \hat{\tau} = \frac{1}{n} \sum_i \phi(X_i, W_i, Y_i)$$



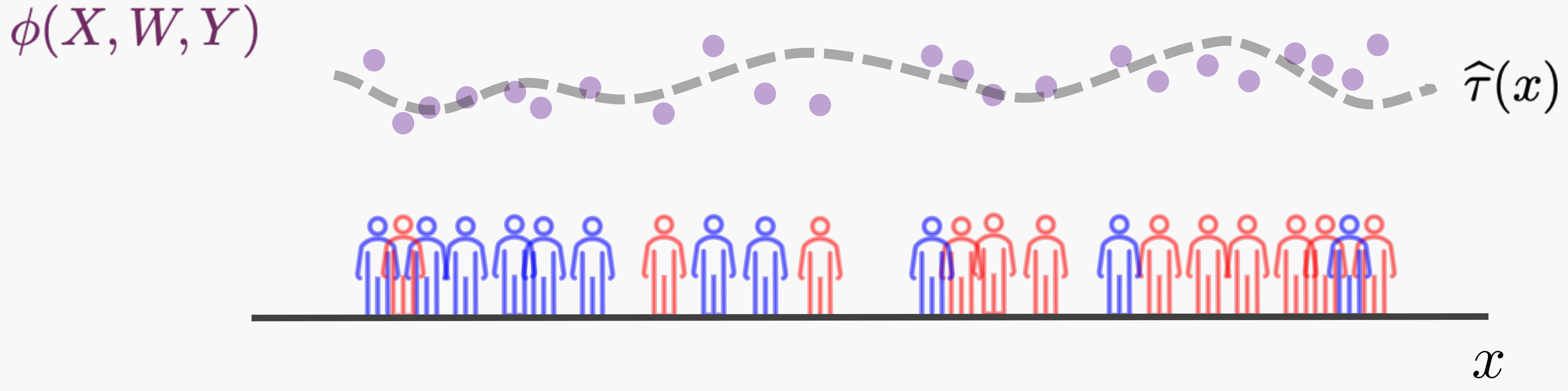
Concept 1: Pseudo-outcome Regression (Meta-learners)

- **Pseudo-outcomes:** Transformations of (X, W, Y) that preserve conditional effects

$$E[\phi(X,W,Y)|X=x] = E[Y(1) - Y(0)|X=x]$$

$$\tau(x) = E[Y(1) - Y(0)|X=x]$$

→ $\hat{\tau}(x)$ **: Regress** $\phi(X,W,Y)$ **on** X



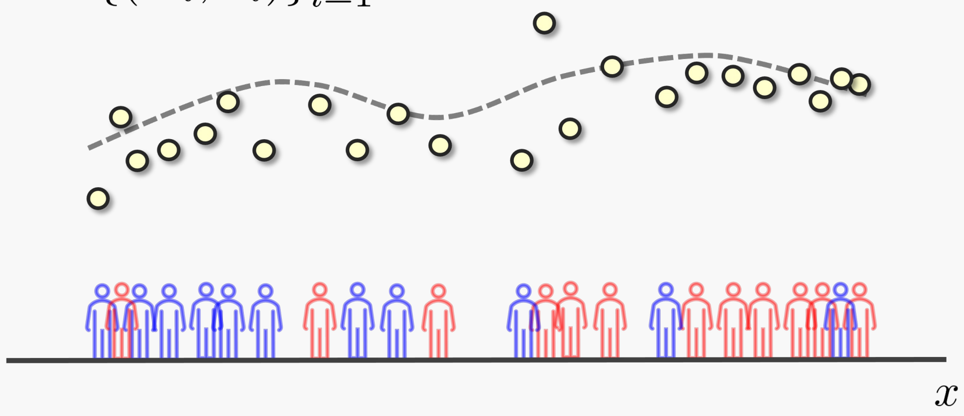
Concept 2: Conformal Prediction

- **Conformal Prediction:** A general approach for **post-hoc** predictive inference (V. Vovk 2012)

Finite-sample validity | Model-free | Distribution-free

Any fitted ML model (point predictions) → Conformal prediction →

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



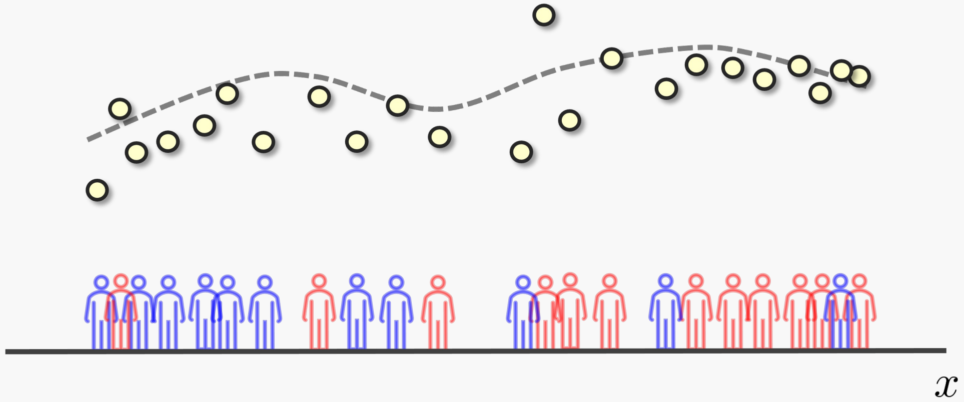
Concept 2: Conformal Prediction

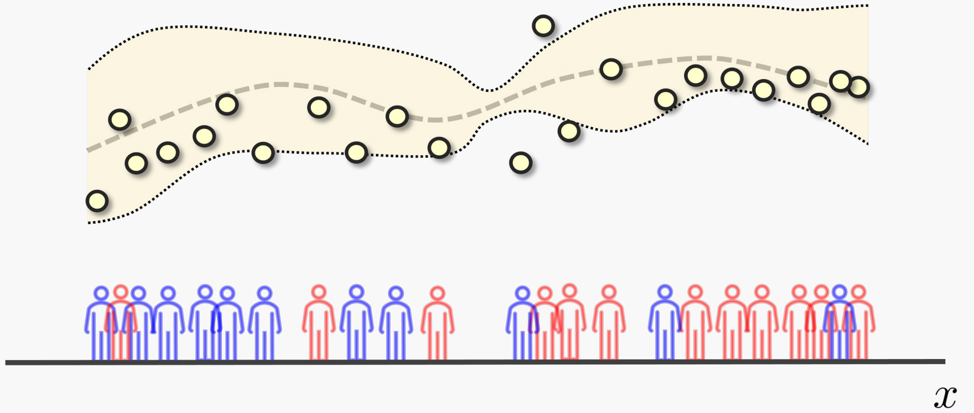
- **Conformal Prediction:** A general approach for **post-hoc** predictive inference (V. Vovk 2012)

Finite-sample validity | Model-free | Distribution-free

Any fitted ML model (point predictions) → Conformal prediction → Valid uncertainty intervals

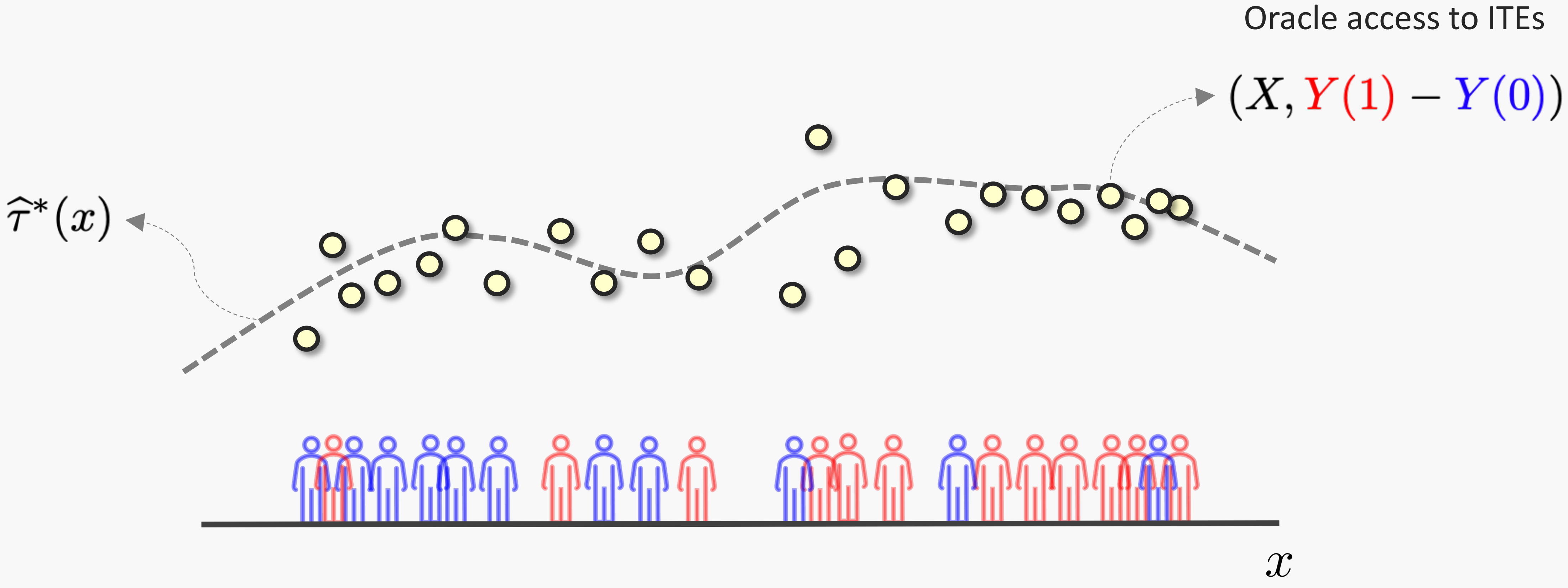
$\{(X_i, Y_i)\}_{i=1}^n$





Concept 2: Conformal Prediction

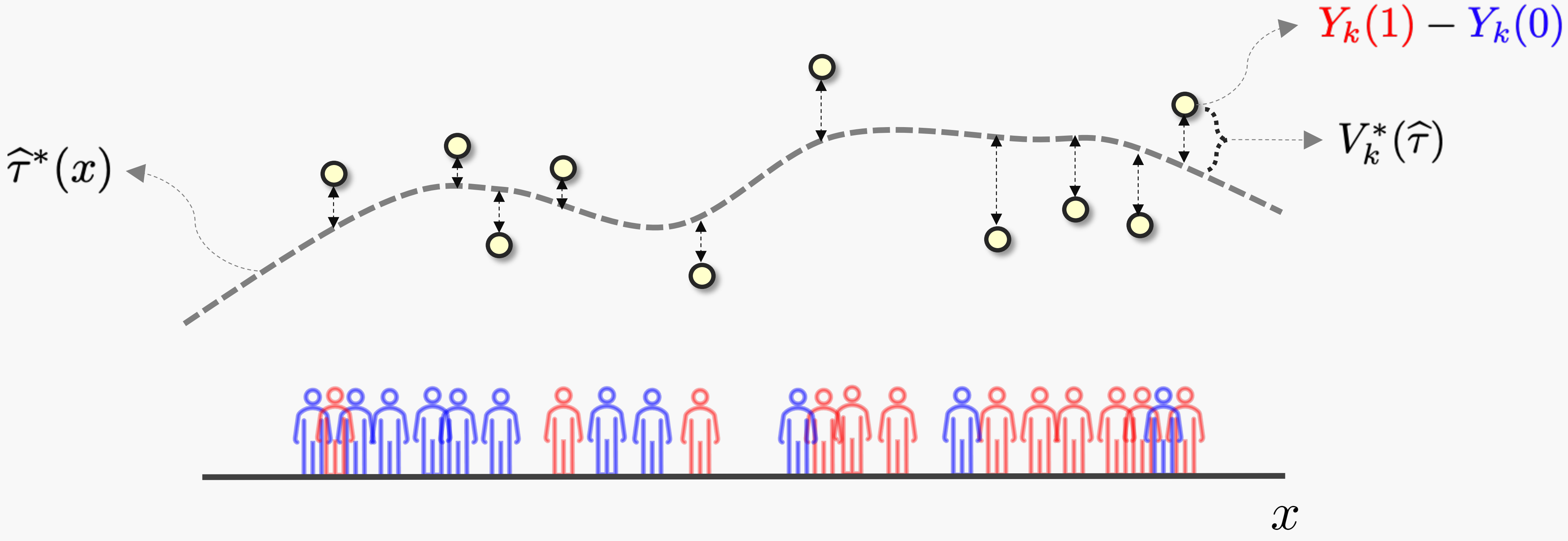
- **Step 1:** Train a machine learning model $\widehat{\tau}^*(x)$ using $\{(X_i, Y_i(1) - Y_i(0))\}_i$



Concept 2: Conformal Prediction

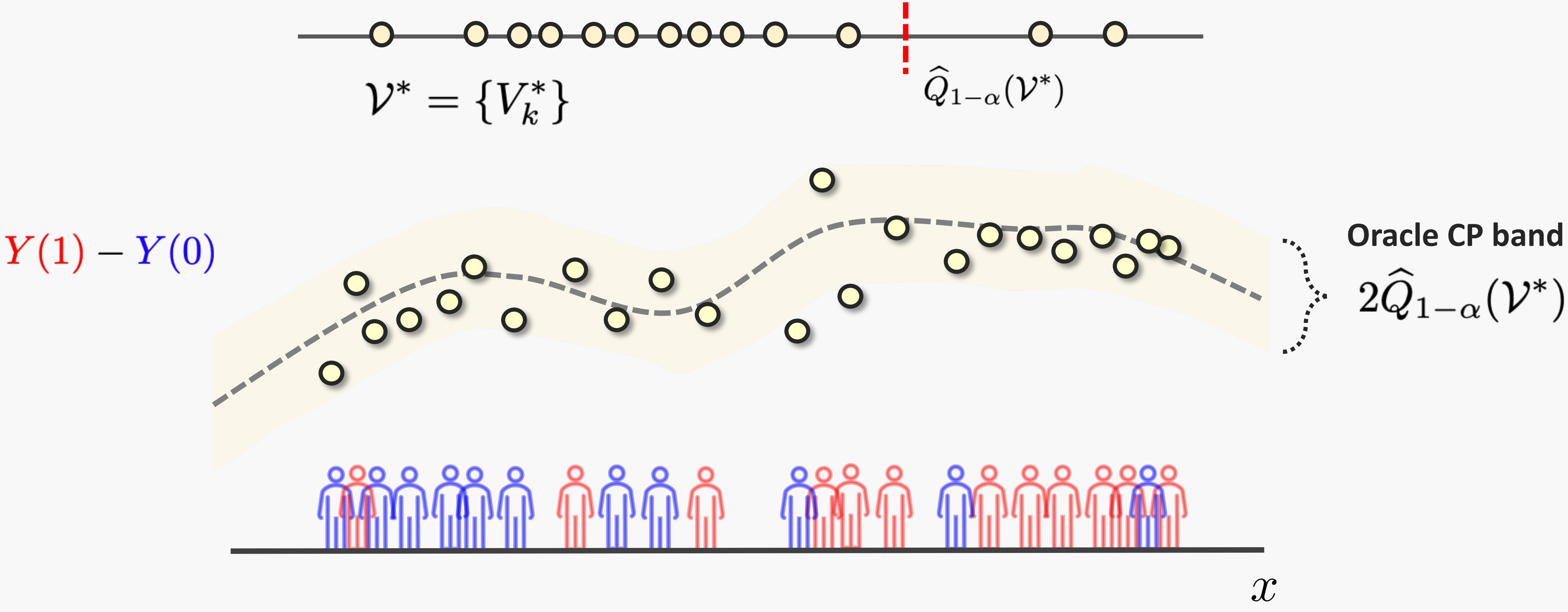
- **Step 2:** Evaluate **conformity scores** on a held-out calibration set

$$V_k^*(\widehat{\tau}) = V(\widehat{\tau}(X_k), Y_k(1) - Y_k(0))$$



Concept 2: Conformal Prediction

- **Step 3:** Construct a predictive interval using the empirical quantile of conformity scores

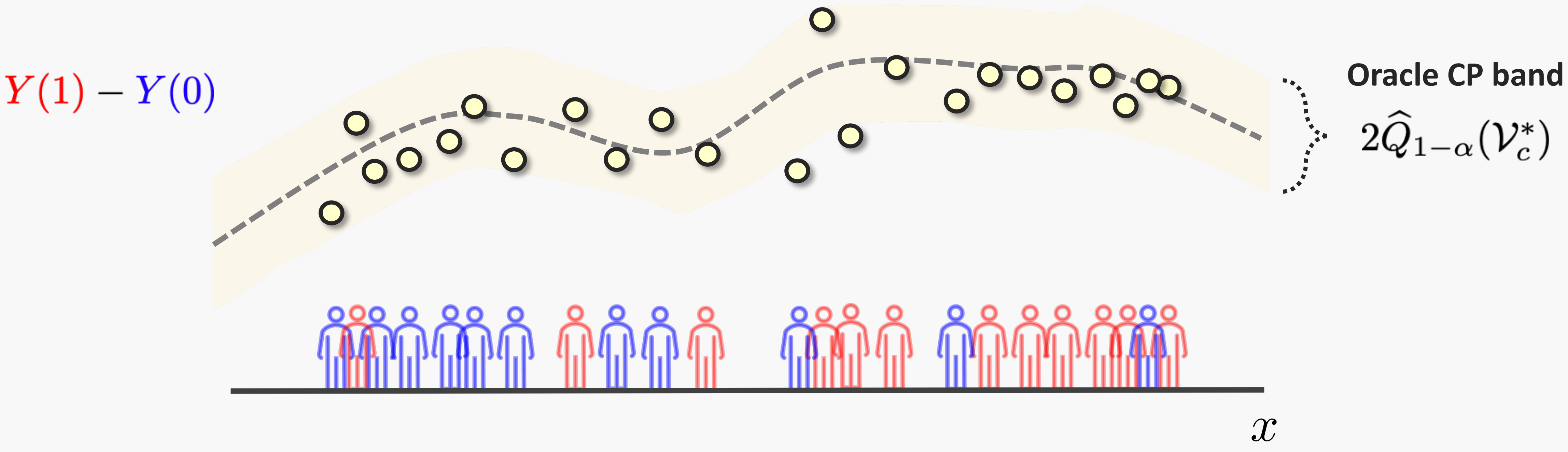


Concept 2: Conformal Prediction

- **Step 3:** Construct a predictive interval using the empirical quantile of conformity scores

$$P(Y_{n+1}(1) - Y_{n+1}(0) \in \widehat{C}^*(X_{n+1})) \geq 1 - \alpha$$

If calibration and test data are exchangeable



Method: Conformal Meta-learners

Concept 1:
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Concept 2:
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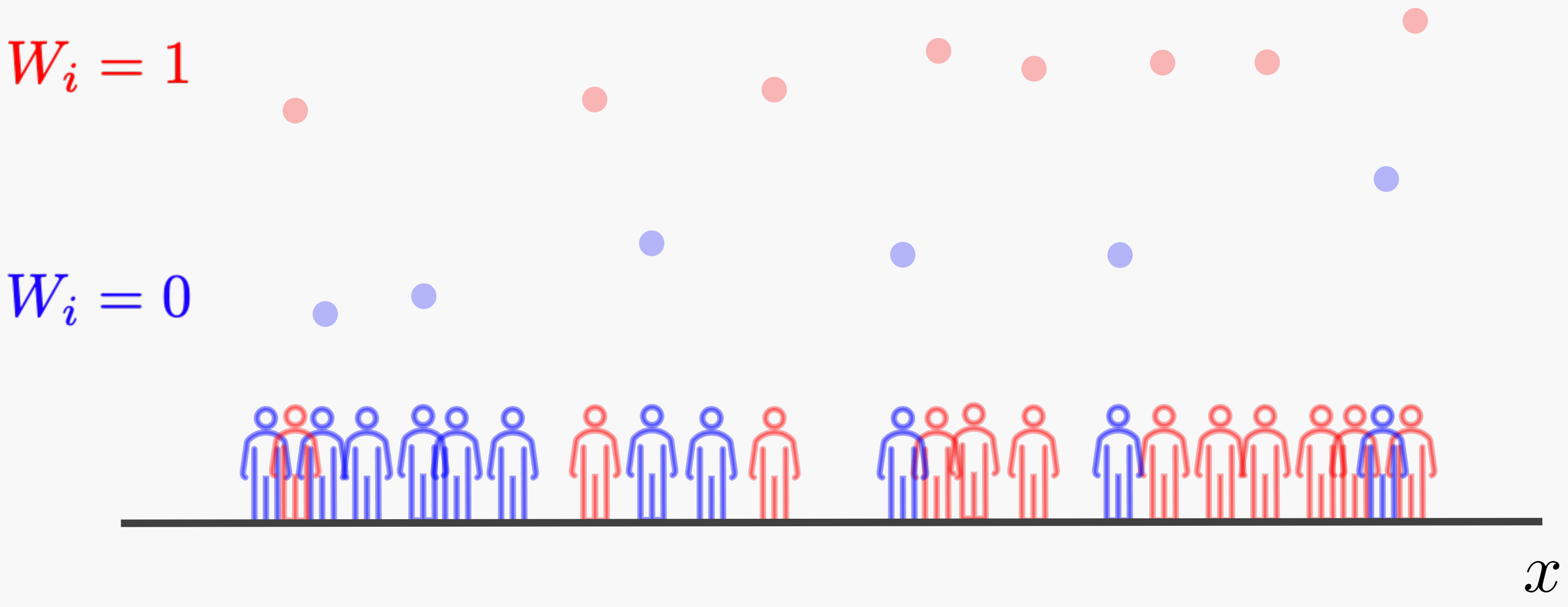
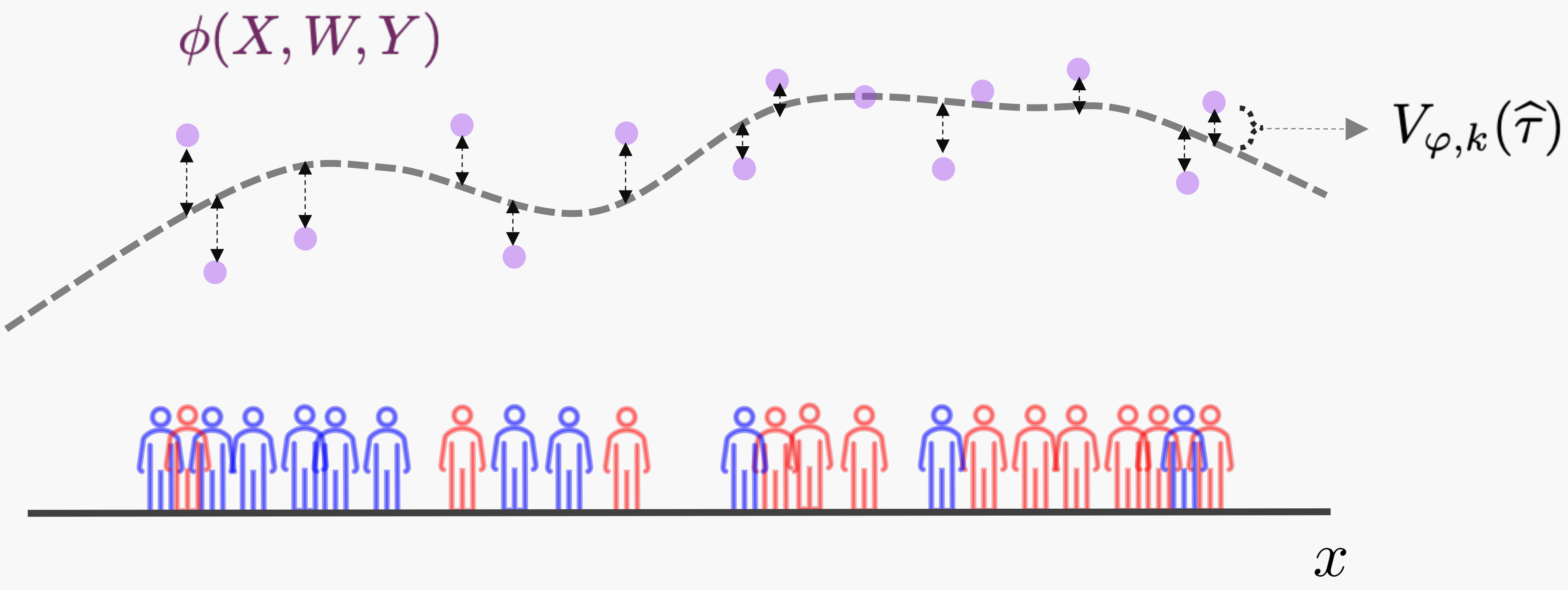


Method: Conformal Meta-learners

- **Key Idea:** Apply CP to pseudo-outcomes instead of unobserved ITEs!

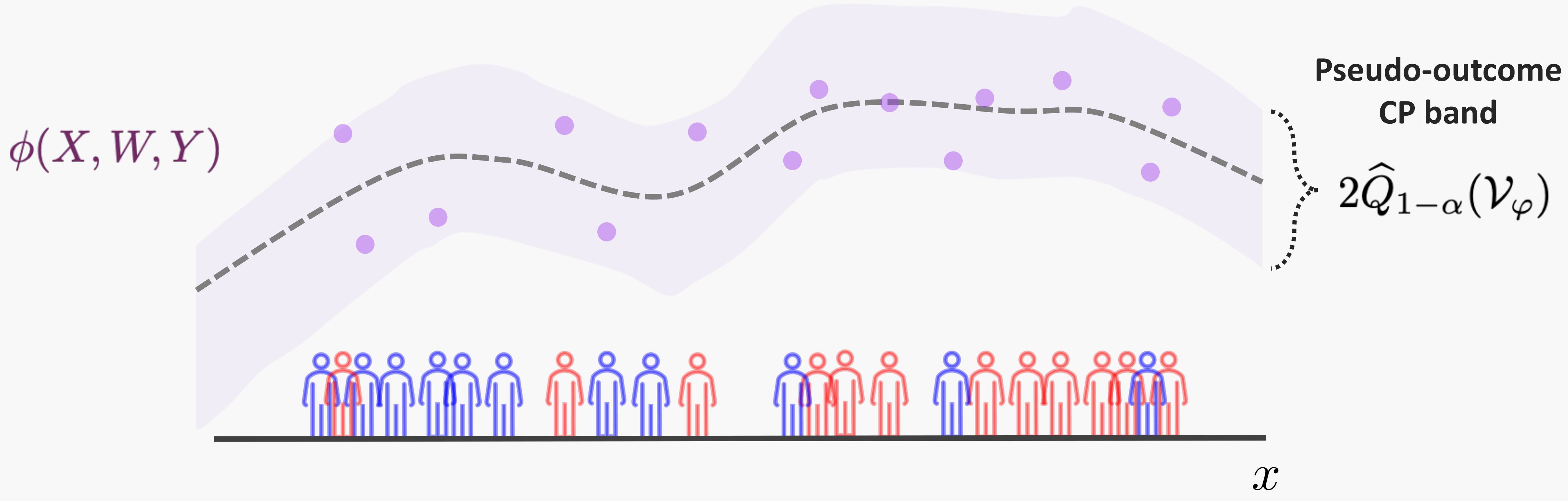
$$V_{\varphi,k}(\widehat{\tau}) = V(\widehat{\tau}(X_k), \phi(X_k, W_k, Y_k))$$



Method: Conformal Meta-learners

- **Key Idea:** Apply CP to pseudo-outcomes instead of unobserved ITEs.

$$P(\phi(X_{n+1}, W_{n+1}, Y_{n+1}) \in \widehat{C}_{\varphi}(X_{n+1})) \geq 1 - \alpha$$

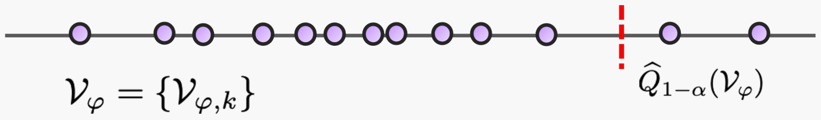


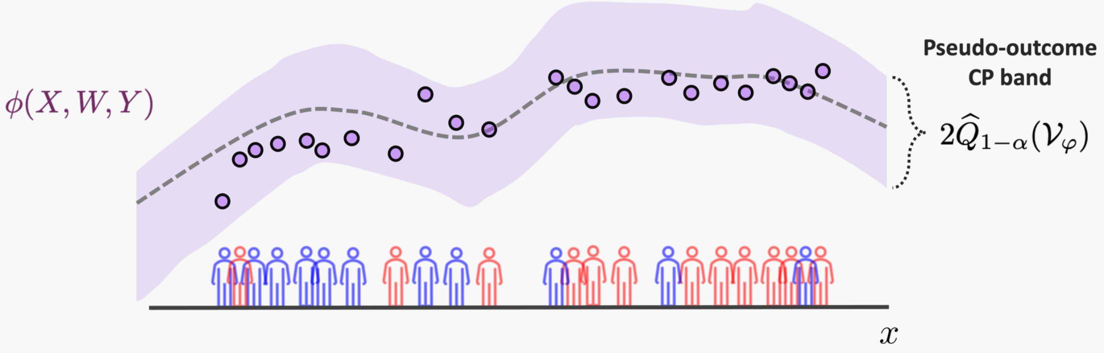
Method: Validity of Meta-learners via Stochastic Ordering Theory

- Under what conditions are predictive intervals for pseudo-outcomes valid for ITEs?

Conformity scores evaluated on pseudo-outcome

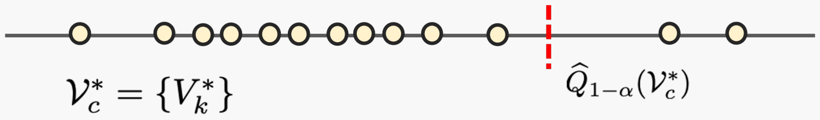
$$V_{\varphi,k}(\widehat{\tau}) = V(\widehat{\tau}(X_k), \phi(X_k, W_k, Y_k))$$

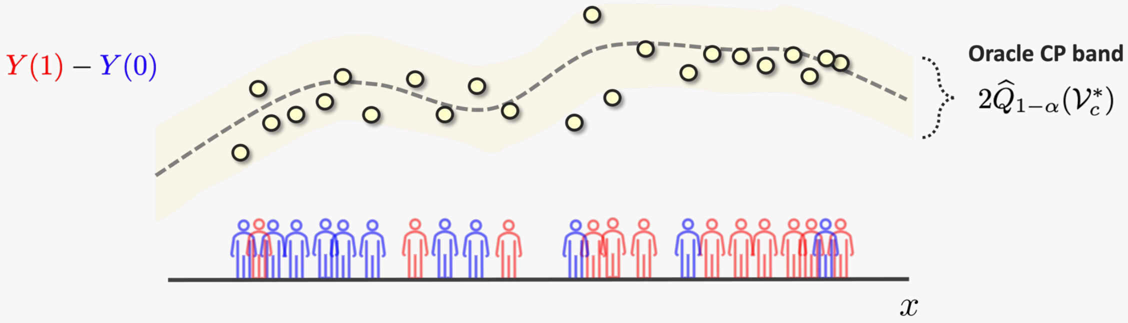




Oracle Conformity scores evaluated on true ITEs

$$V_k^*(\widehat{\tau}) = V(\widehat{\tau}(X_k), Y_k(1) - Y_k(0))$$

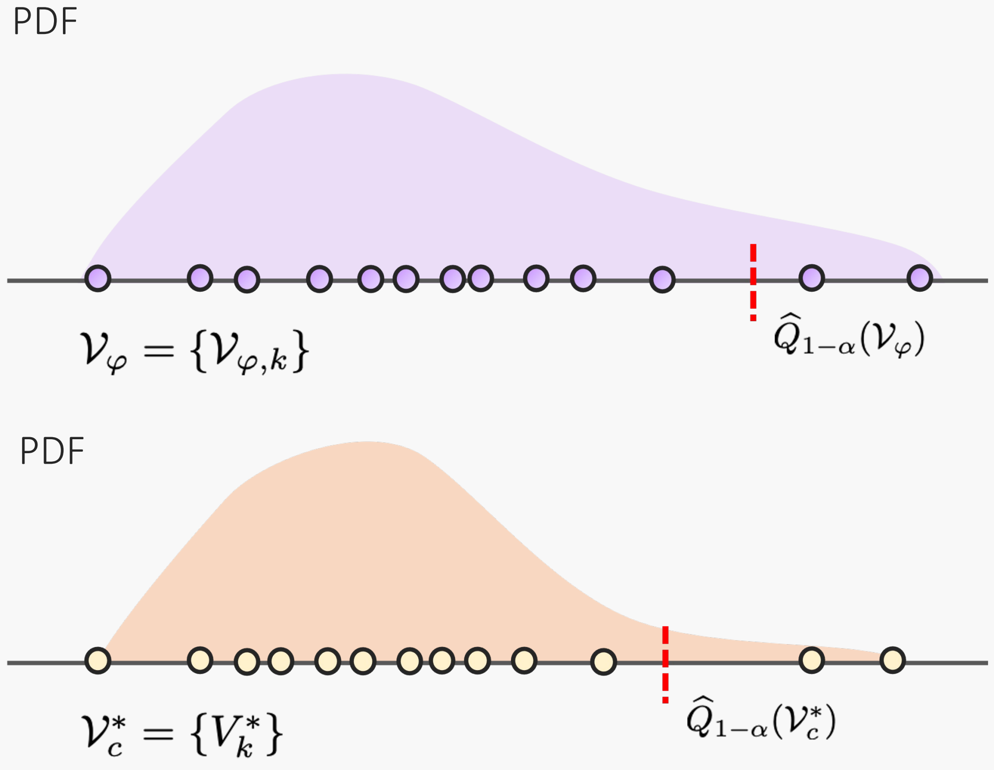


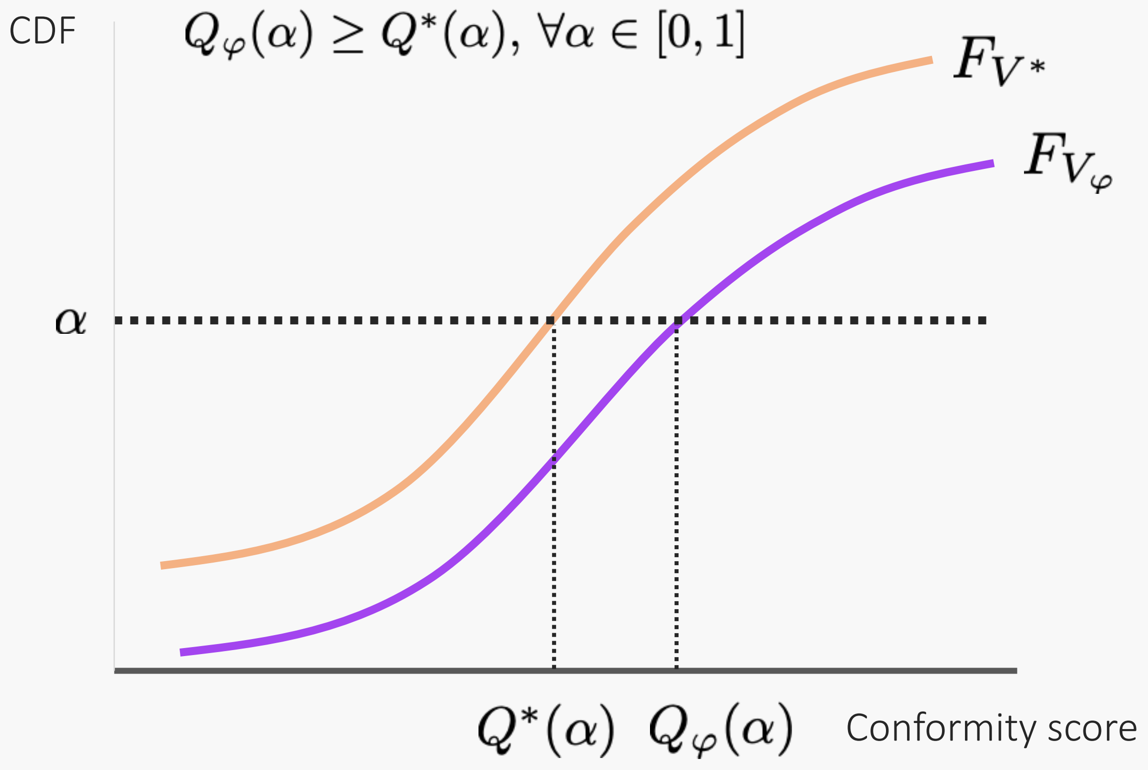


Method: Validity of Meta-learners via Stochastic Ordering Theory

- **Sufficient condition for validity:** First-order stochastic dominance!

$$V_{\varphi}(\widehat{\tau}) \succeq V^{*}(\widehat{\tau})$$





Method: Validity of Meta-learners via Stochastic Ordering Theory

- Unified analysis of validity of meta-learners = stochastic orders of $V_\varphi(\widehat{\tau})$ and $V^*(\widehat{\tau})$

Meta-learner	Pseudo-outcome
X-learner	$\phi_{\mathrm{X}} = W(Y - \widehat{\mu}_0(X)) + (1-W)(\widehat{\mu}_1(X) - Y)$
IPW-learner Inverse propensity weighted	$\phi_{\mathrm{IPW}} = \frac{W-\pi(X)}{\pi(X)(1-\pi(X))} Y$
DR-learner Doubly-robust learner	$\phi_{\mathrm{DR}} = \frac{W-\pi(X)}{\pi(X)(1-\pi(X))}(Y - \widehat{\mu}_W(X)) + (\widehat{\mu}_1(X) - \widehat{\mu}_0(X))$

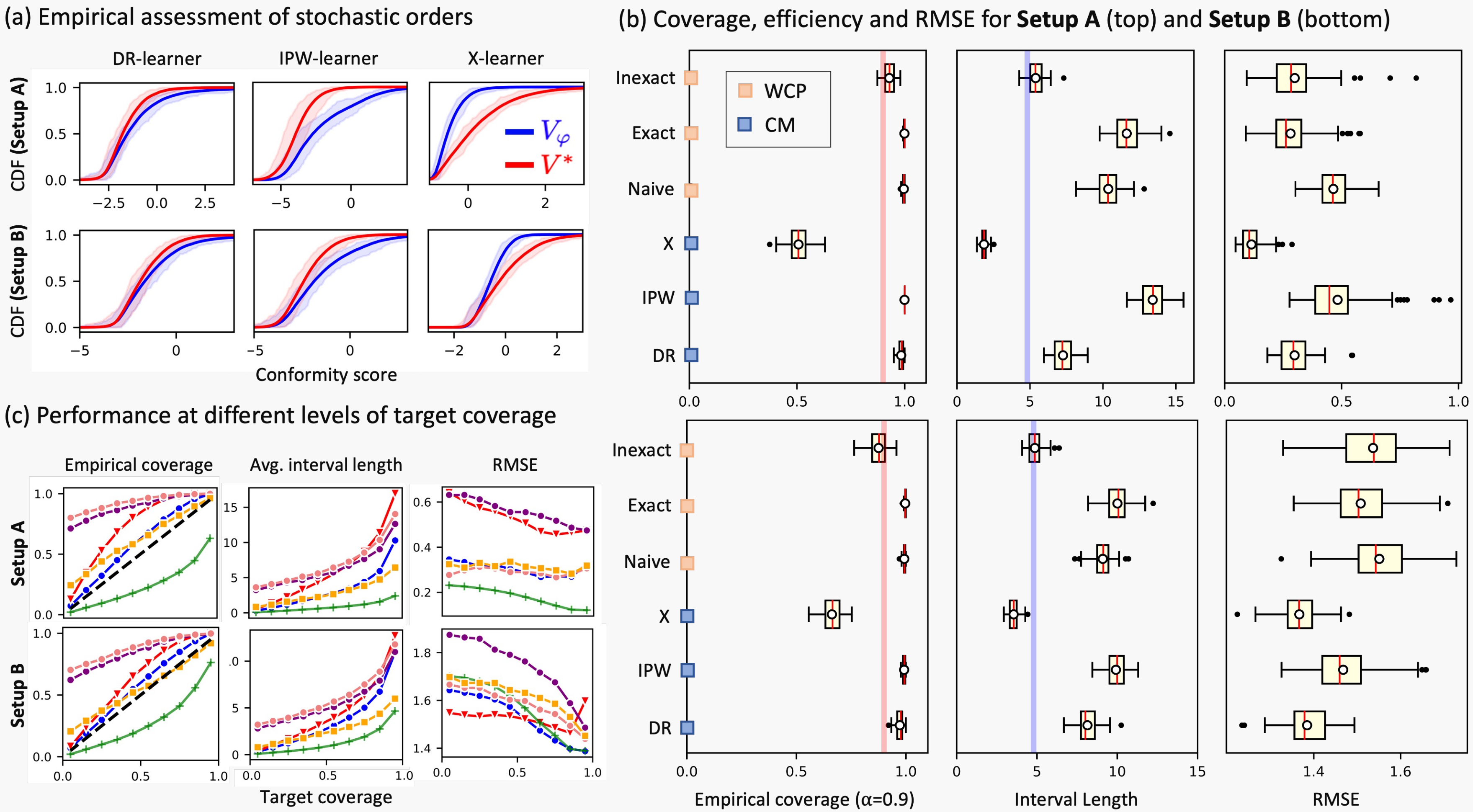
Method: Validity of Meta-learners via Stochastic Ordering Theory

- Commonly-used meta-learners guarantee model-/distribution-free stochastic orders!

Meta-learner	Stochastic orders of Conformity Scores
X-learner	No distribution-free stochastic order!
IPW-learner Inverse propensity weighted	$V^* \succeq_{(2)} V_{\mathrm{IPW}}$
DR-learner Doubly-robust learner	$V^* \succeq_{(2)} V_{\mathrm{DR}}$

Results and Takeaway

- **TL;DR: Conformal meta-learners =** valid predictive inference + accurate point predictions



Poster Session 2

Tuesday Dec. 12

5:15 pm – 7:15 pm