Approximate Conditional Coverage via Neural Model Approximations

Allen Schmaltz and Danielle Rasooly

Reexpress AI, Inc. and Harvard University

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5 minute overview

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Desiderata for deploying deep learning models

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- Interpretability
  - Map: Relevant feature subsets to those with known labels
- Local updatability
- Uncertainty quantification

We seek a general framework with all of these properties

Desiderata for uncertainty quantification

- Minimize distributional assumptions
- Robustness to data shifts (covariate & label shift)
- Out-of-distribution data does not lead to unexpected catastrophes
- Minimize free parameters (i.e., practical reliability)
- Informative coverage
  - Prefer conservative coverage over under-coverage

Split-conformal prediction sets for classification

- Computationally expensive blackbox: F
- Training dataset: $\mathscr{D}_{\text{tr}} = \{(X_i, Y_i)\}_{i=1}^{I}$ with $Y_i \in \mathscr{Y} = \{1, \ldots, C\}$
- Held-out labeled calibration dataset: $\mathscr{D}_{\text{ca}} = \{(X_j, Y_j)\}_{j=I+1}^{N=I+J}$

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- Finite-sample *marginal* guarantee:
    - $\mathbb{P}\left\{ Y_{N+1} \in \hat{\mathscr{C}}(X_{N+1}) \right\} \geq 1 - \alpha$
    - Via $\hat{\mathscr{C}}(x_{N+1}) = \left\{ c \in \mathscr{Y} : \hat{\pi}^c(x_{N+1}) \geq \hat{\tau}^{\alpha} \right\}$, where $\hat{\tau}^{\alpha} = 1 - \hat{l}^{\alpha}$

Quantile threshold

conditional coverage

- Finite-sample *conditional* coverage:

$$\mathbb{P}\left\{Y_{N+1} \in \hat{\mathscr{C}}(X_{N+1}) \mid X_{N+1} = x\right\} \geq 1 - \alpha$$

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Approximate conditional coverage

- Finite-sample *conditional* coverage:

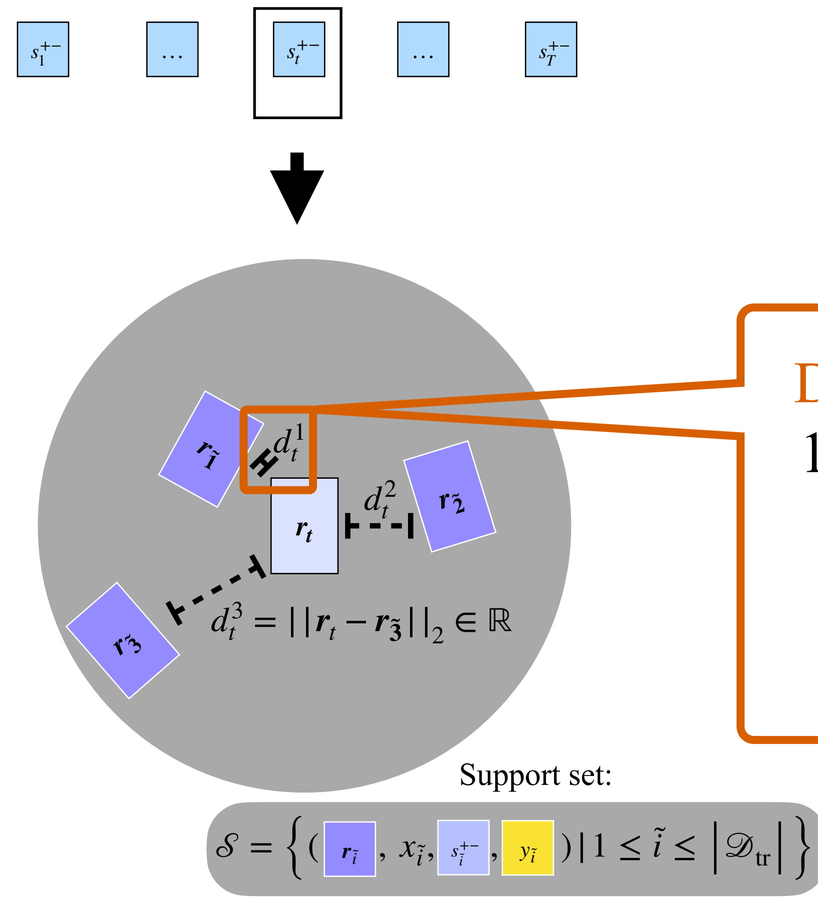
$$\mathbb{P}\left\{ Y_{N+1} \in \hat{\mathscr{C}}(X_{N+1}) \mid X_{N+1} = x \right\} \geq 1 - \alpha$$

- Finite-sample *approximate conditional* coverage:

$$\mathbb{P}\left\{ Y_{N+1} \in \hat{\mathscr{C}}(X_{N+1}) \mid X_{N+1} \in \mathscr{B}(x), Y_{N+1} = y \right\} \geq 1 - \alpha, \text{ with } P_X(\mathscr{B}(x)) \geq \xi$$

Recast a prediction as a weighting over the training set

KNN Approximation

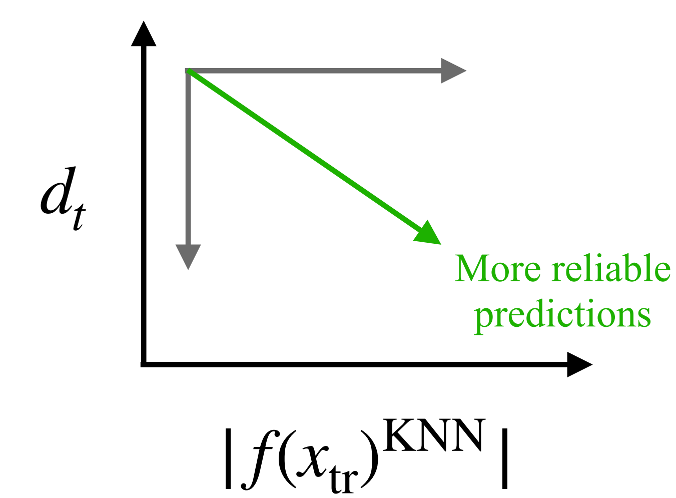


Data uncertainty: Distance to 1st match (d_t), an exogenous factor, captures uncertainty w.r.t. data (training data compared to test data).

Model uncertainty: This bounded value reaches its min/max when $\tanh(s_k^{+-})$ & y (or y_k, with token-level labels) agree, for all k (assuming $\gamma > 0$).

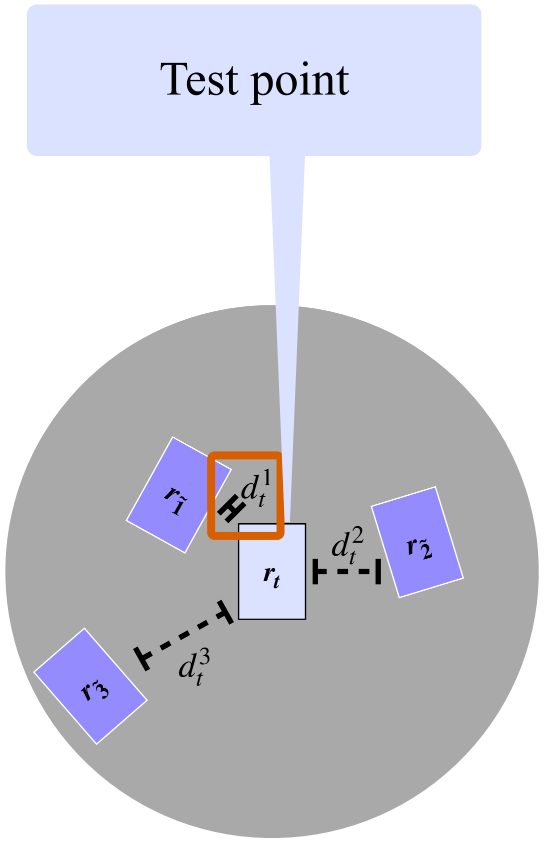
$$
\begin{aligned}
s_t^{+-} \approx \beta &+ w_1 \cdot \left(\tanh(s_{\tilde1}^{+-}) + \gamma \cdot y_{\tilde1}\right) \\
&+ w_2 \cdot \left(\tanh(s_{\tilde2}^{+-}) + \gamma \cdot y_{\tilde2}\right) \\
&+ w_3 \cdot \left(\tanh(s_{\tilde3}^{+-}) + \gamma \cdot y_{\tilde3}\right)
\end{aligned}
$$

$$
w_k = \frac{\exp(-d_k/\eta)}{\sum_{k'=1}^{3} \exp(-d_{k'}/\eta)}
$$

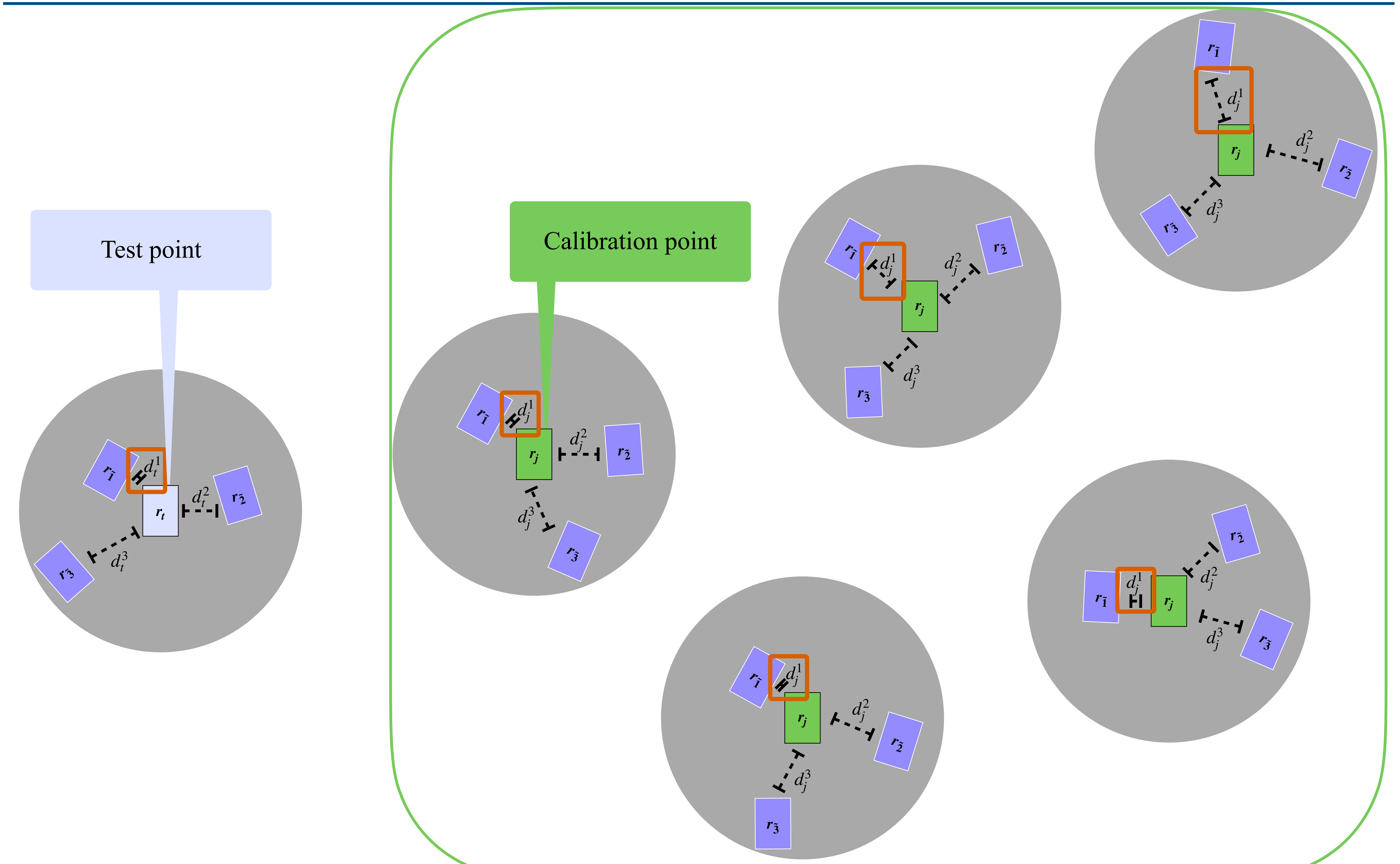


Magnitude of the K-NN Output

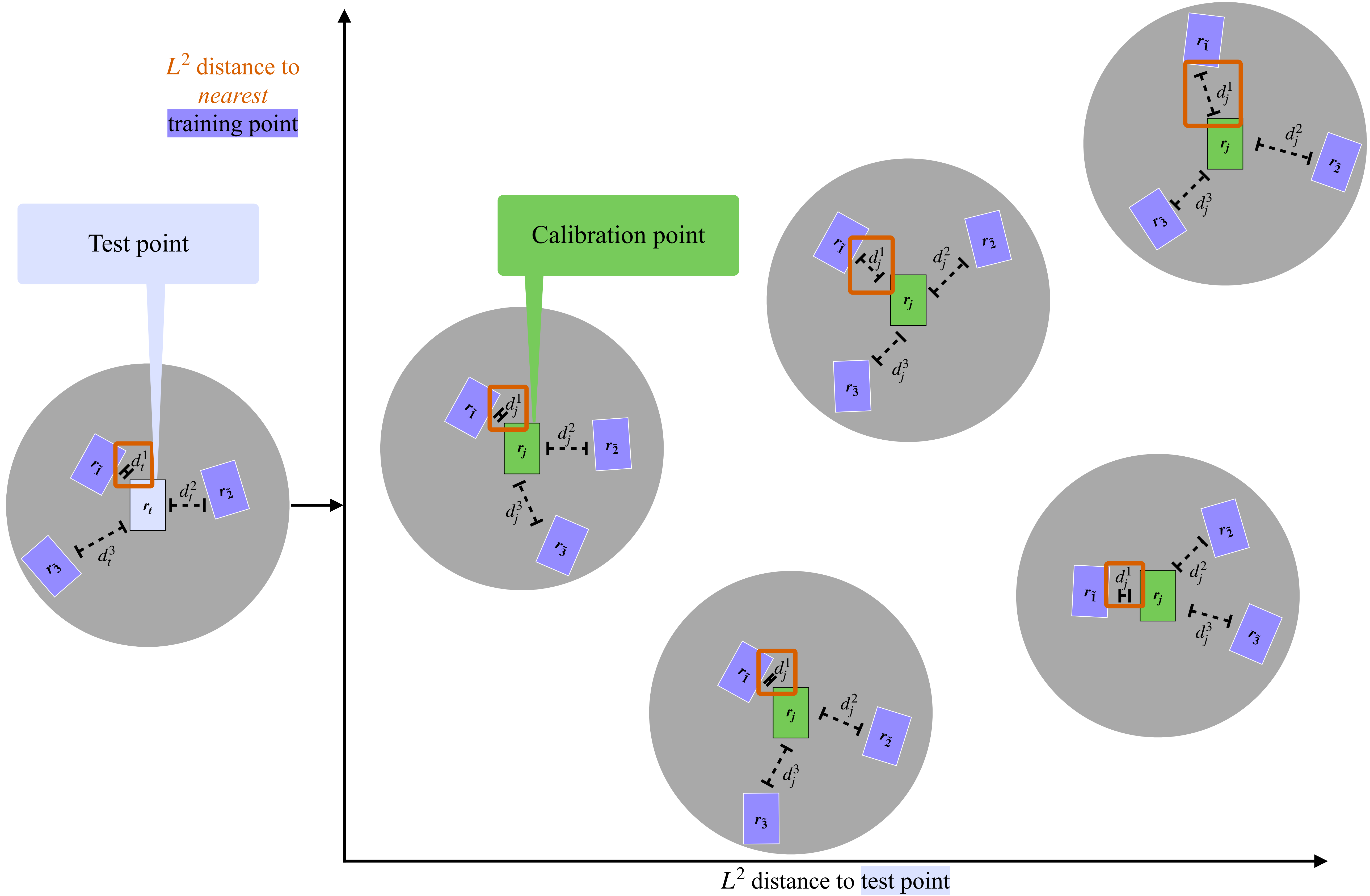
Construct approximation for test point



Construct approximation for test point and all calibration points



Relate test point to distribution of calibration points



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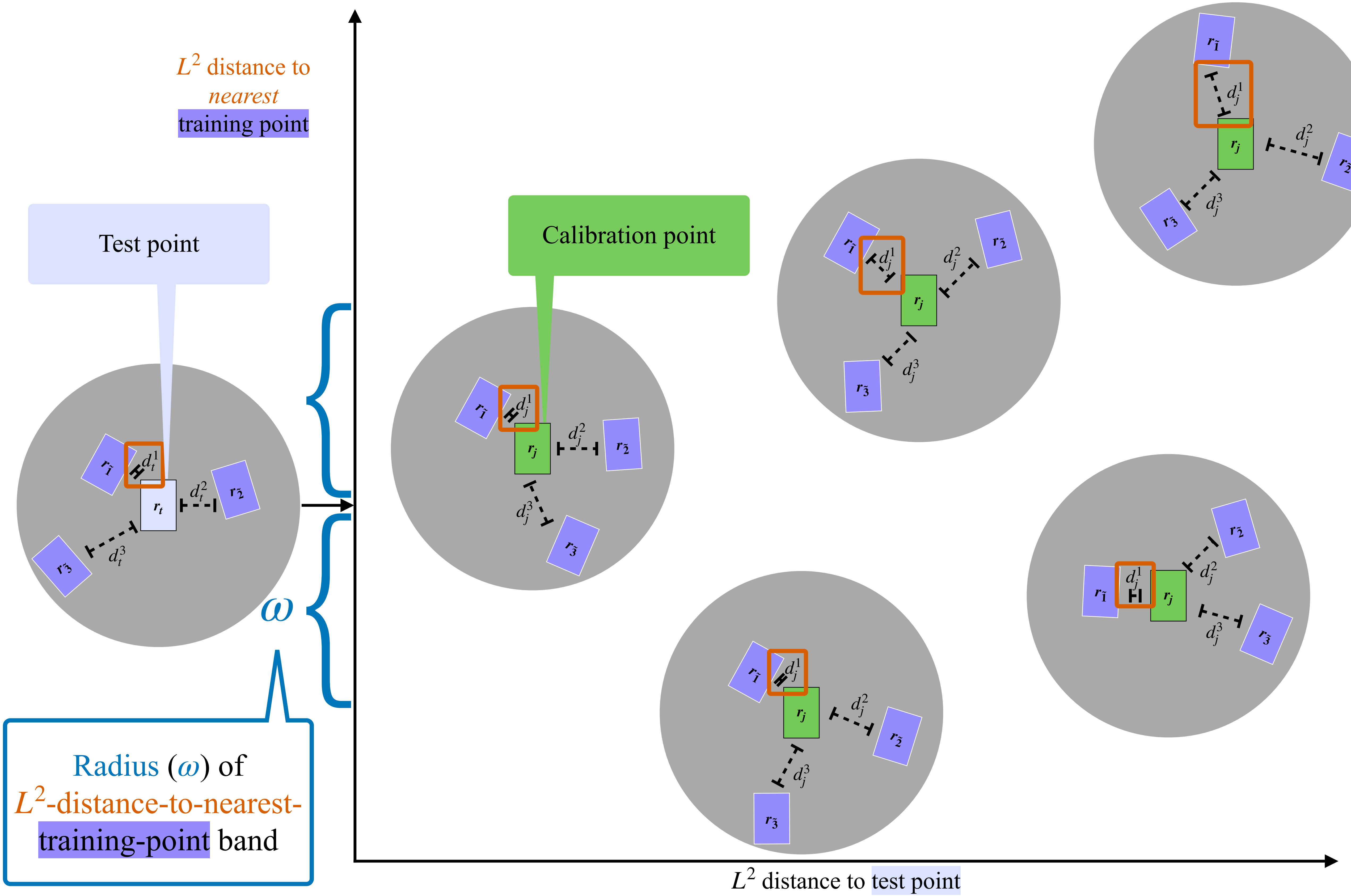
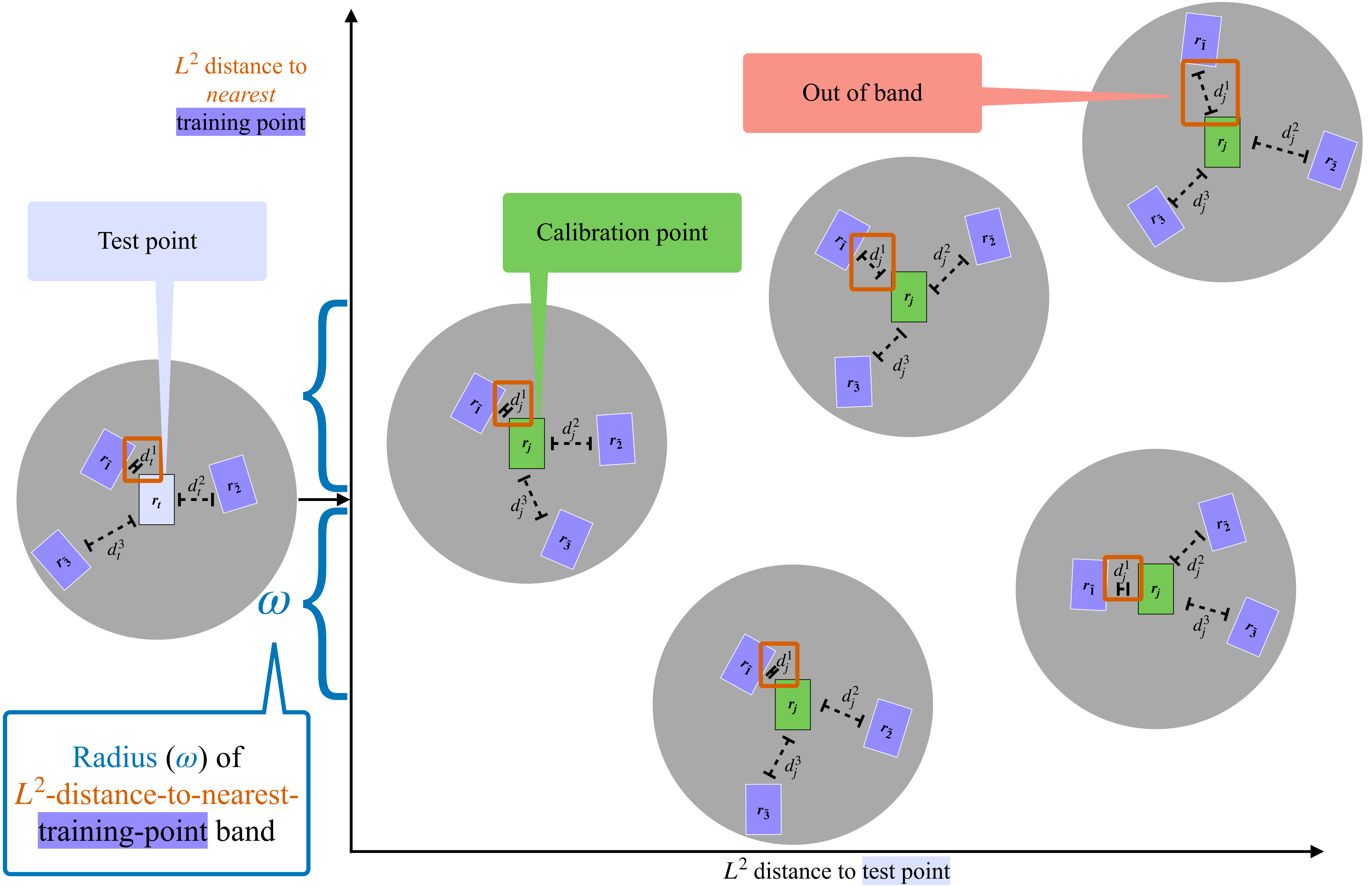
Construct a distance band around the test point



Constrain calibration points to distance band



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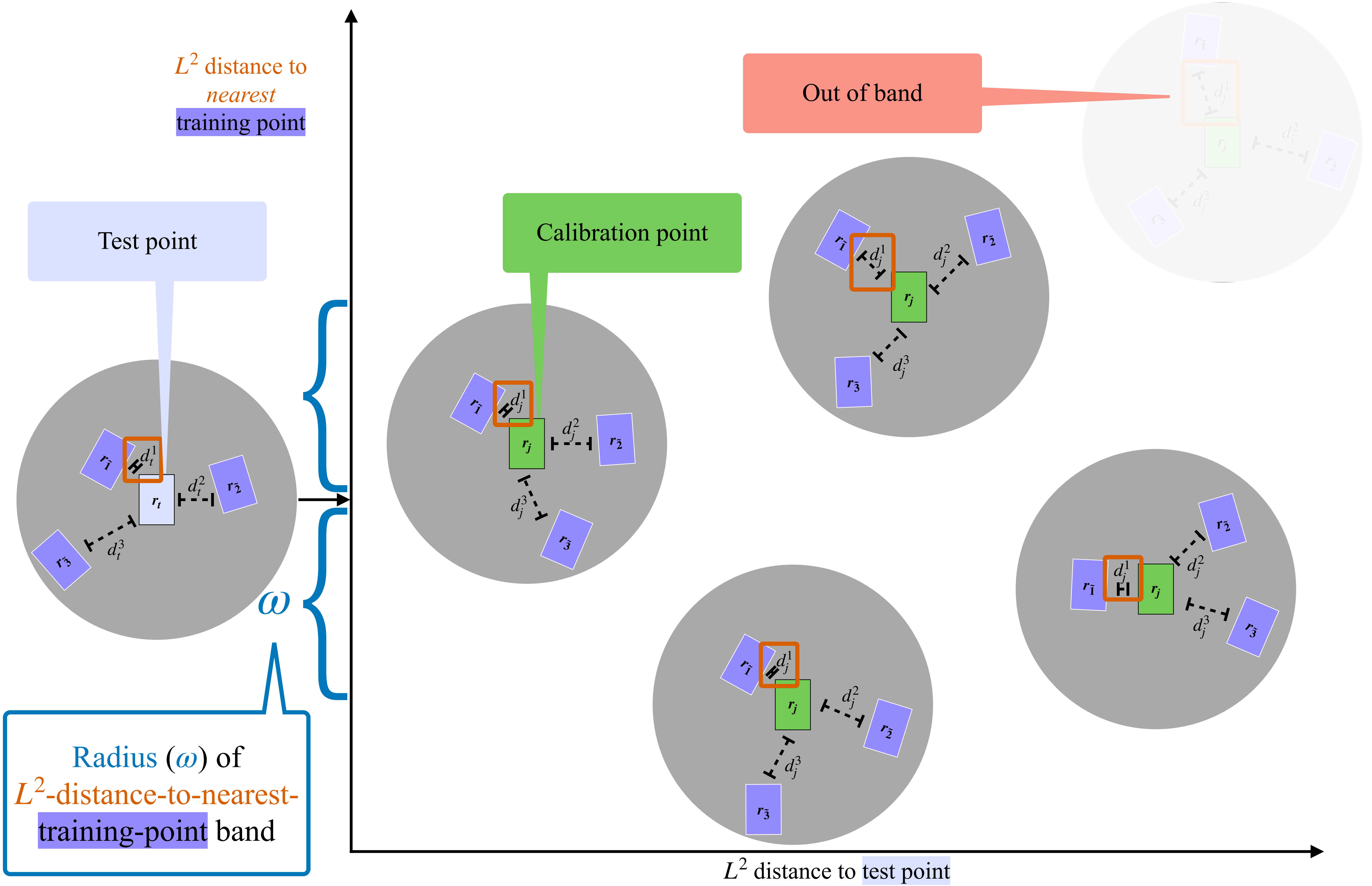

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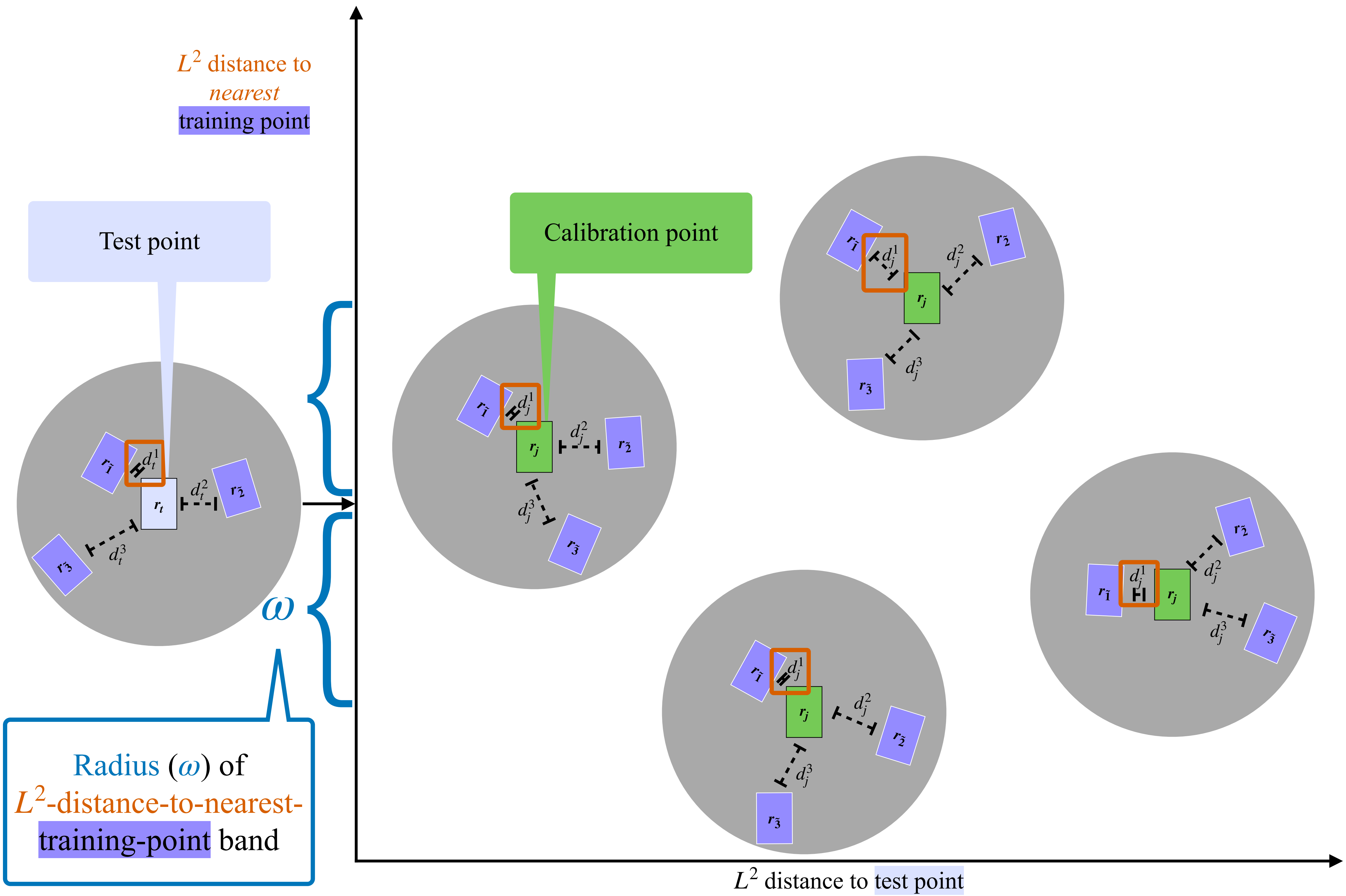
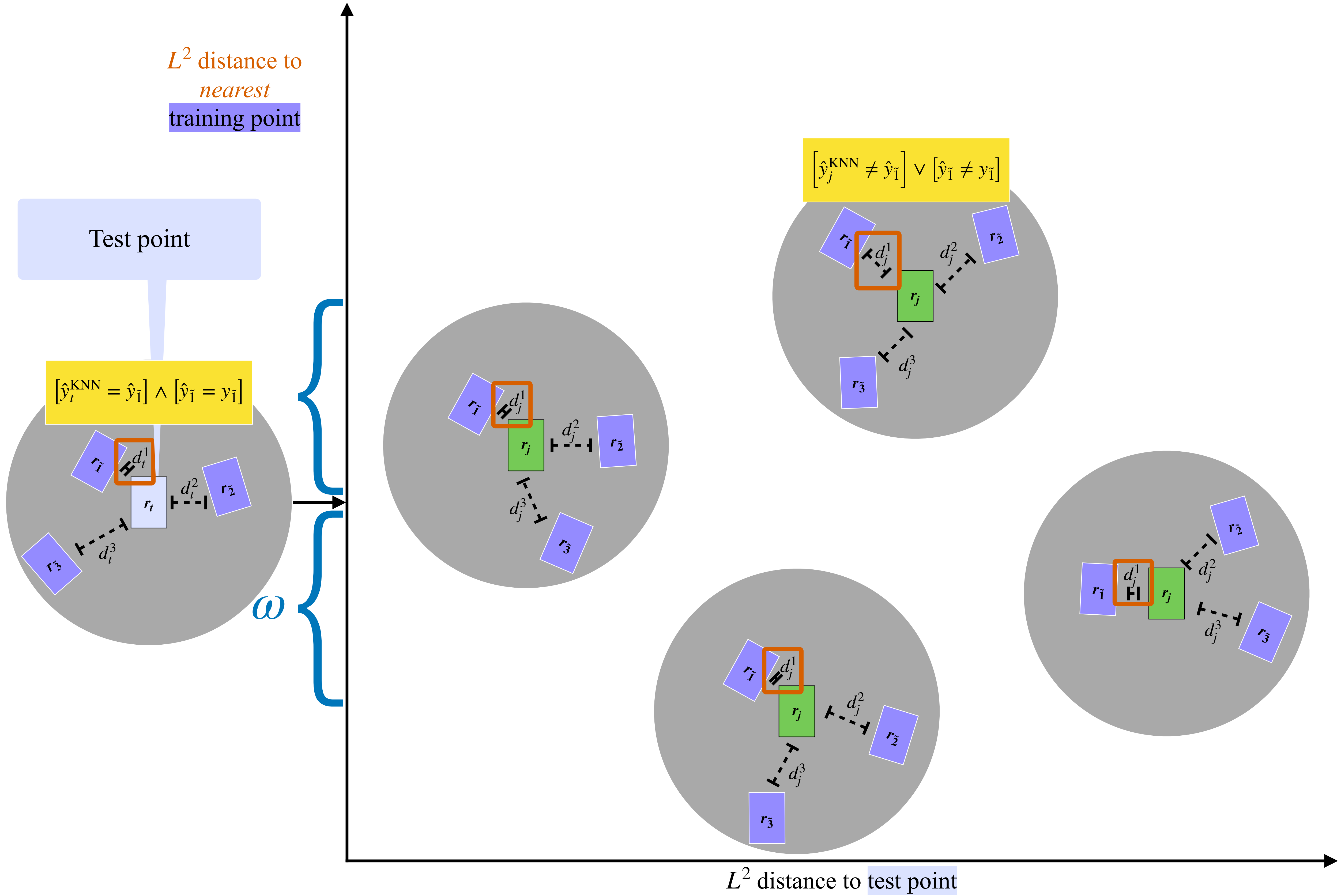
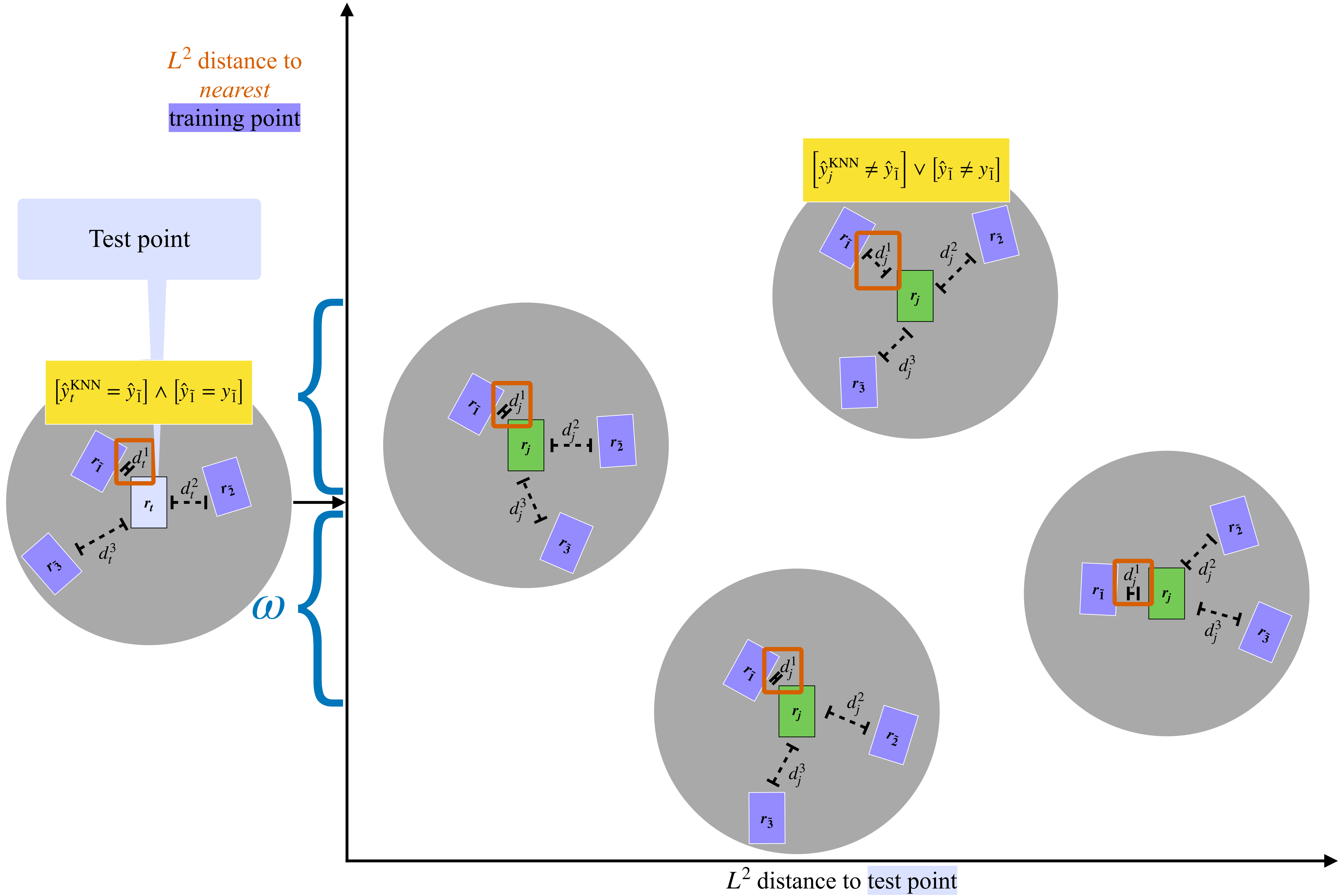


match constraint feature



Constrain calibration points to match constraint feature



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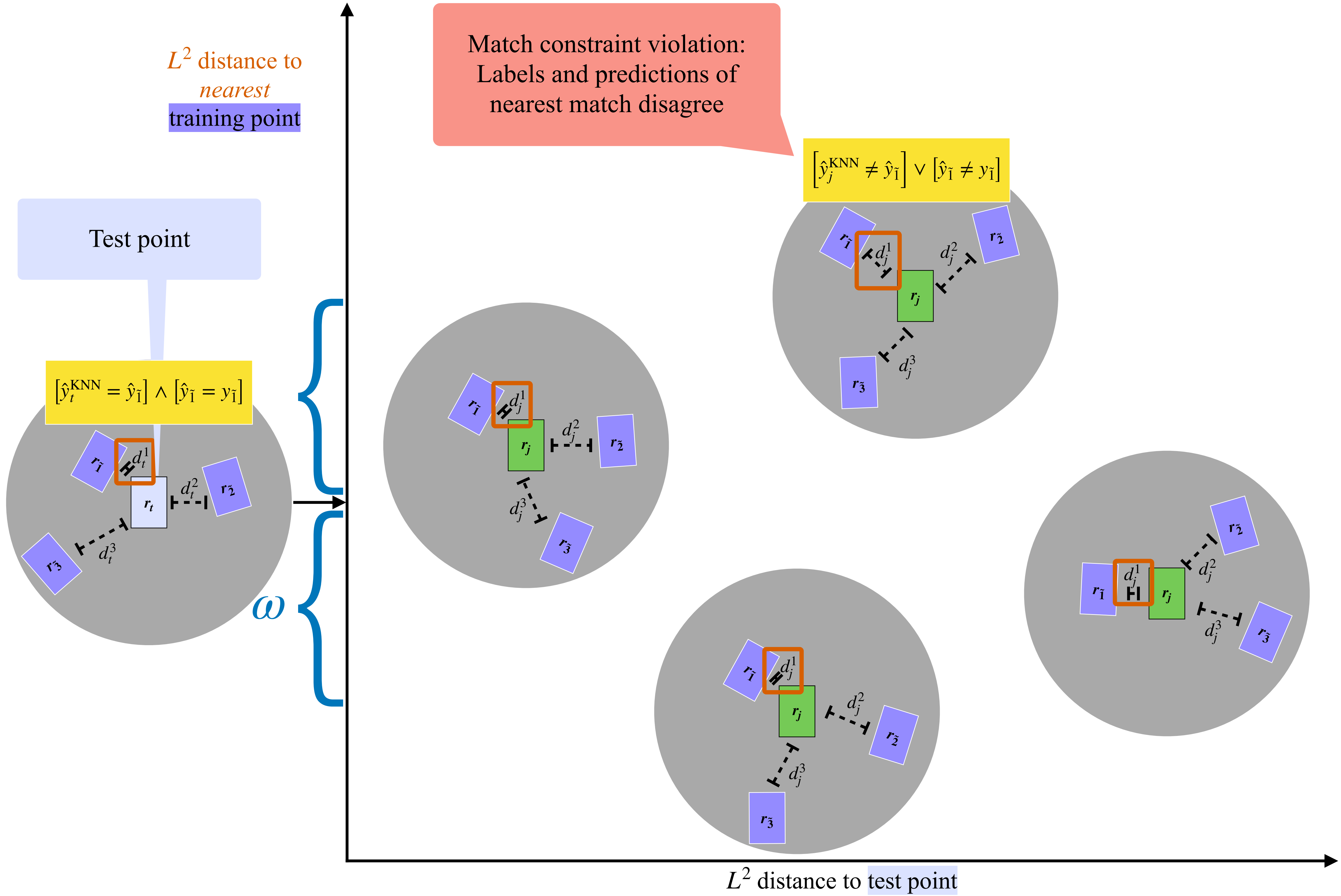

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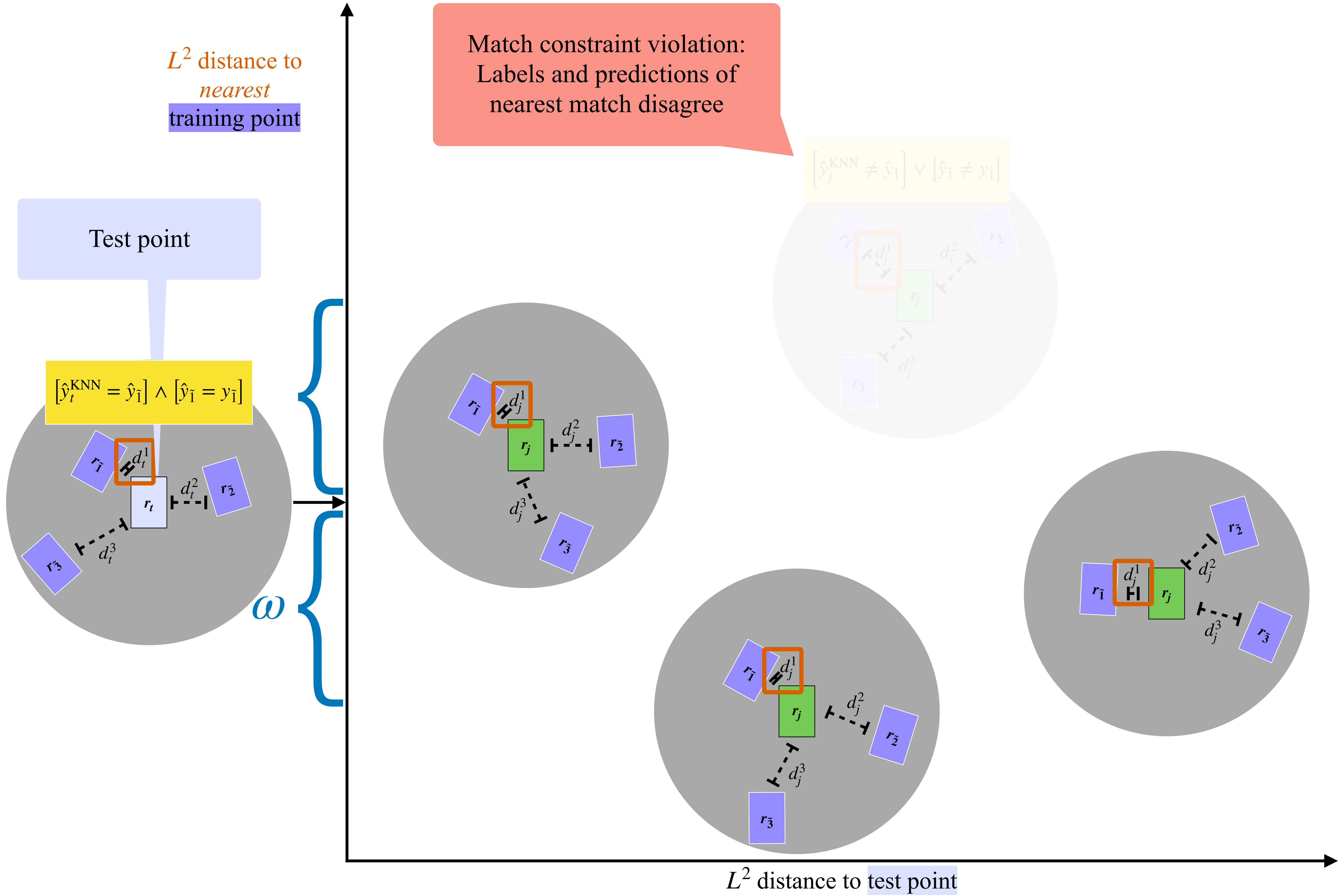

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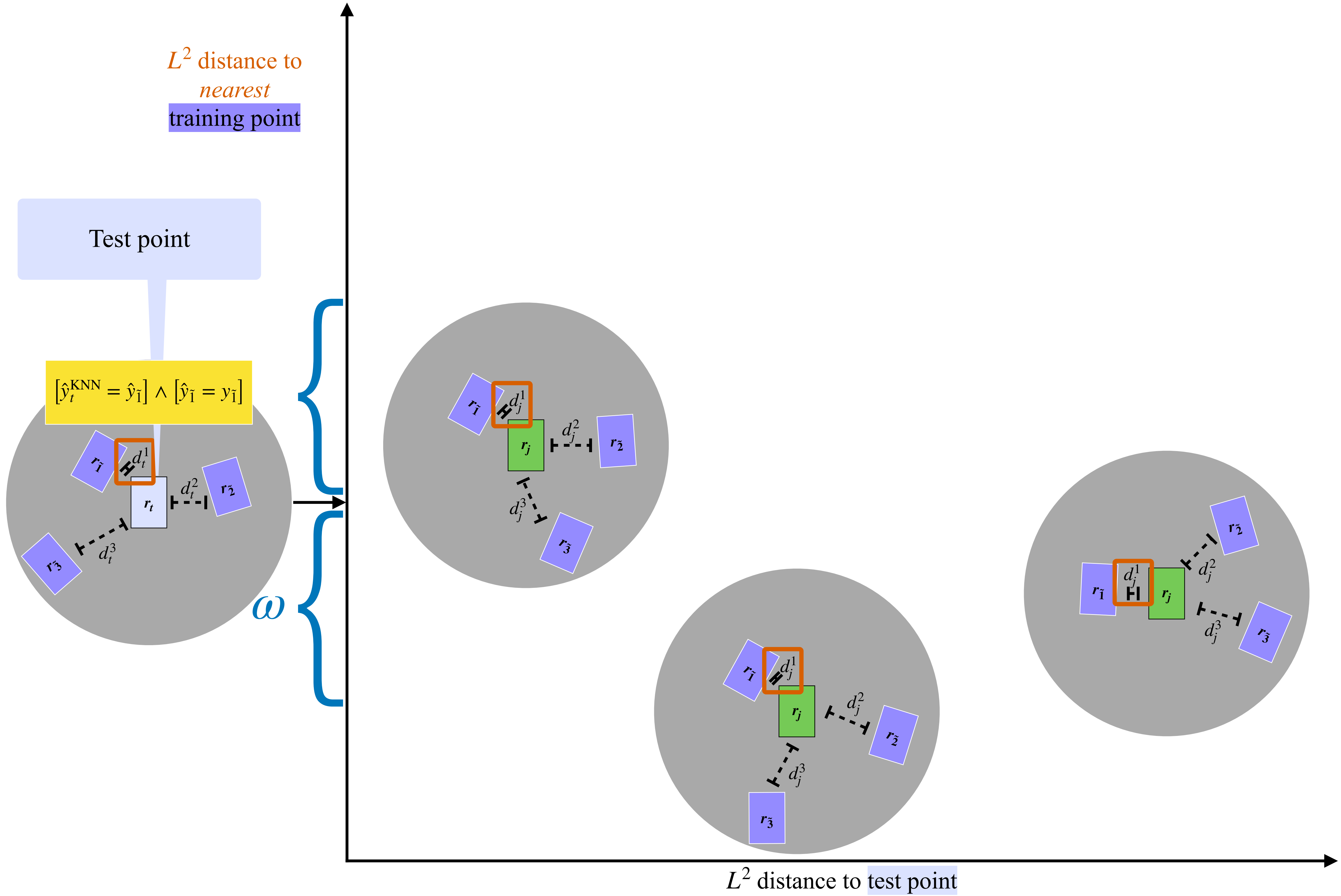
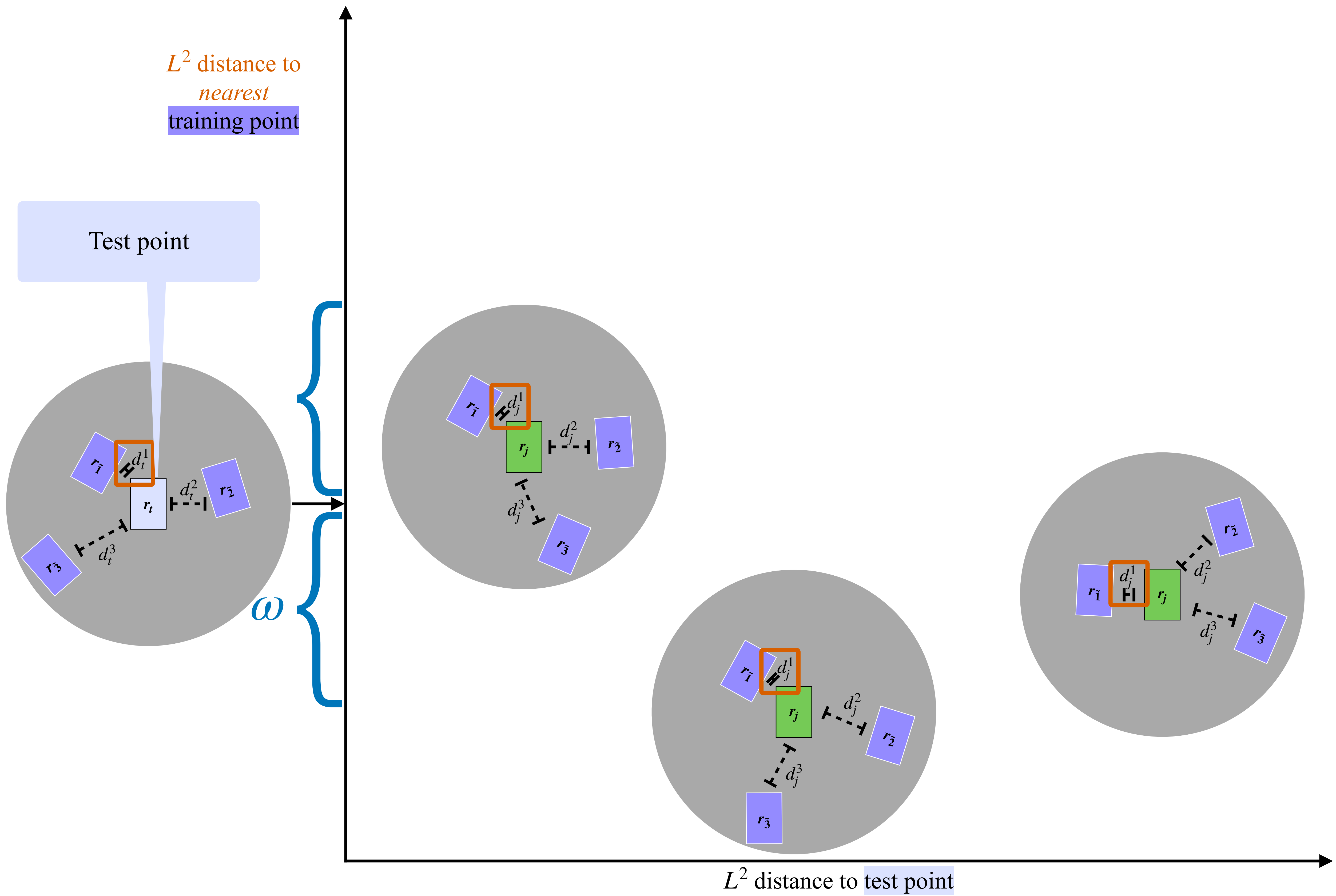


Re-sample $\mathscr{D}_{\mathrm{ca}}$ to be more similar to $\mathscr{D}_{\mathrm{te}}$



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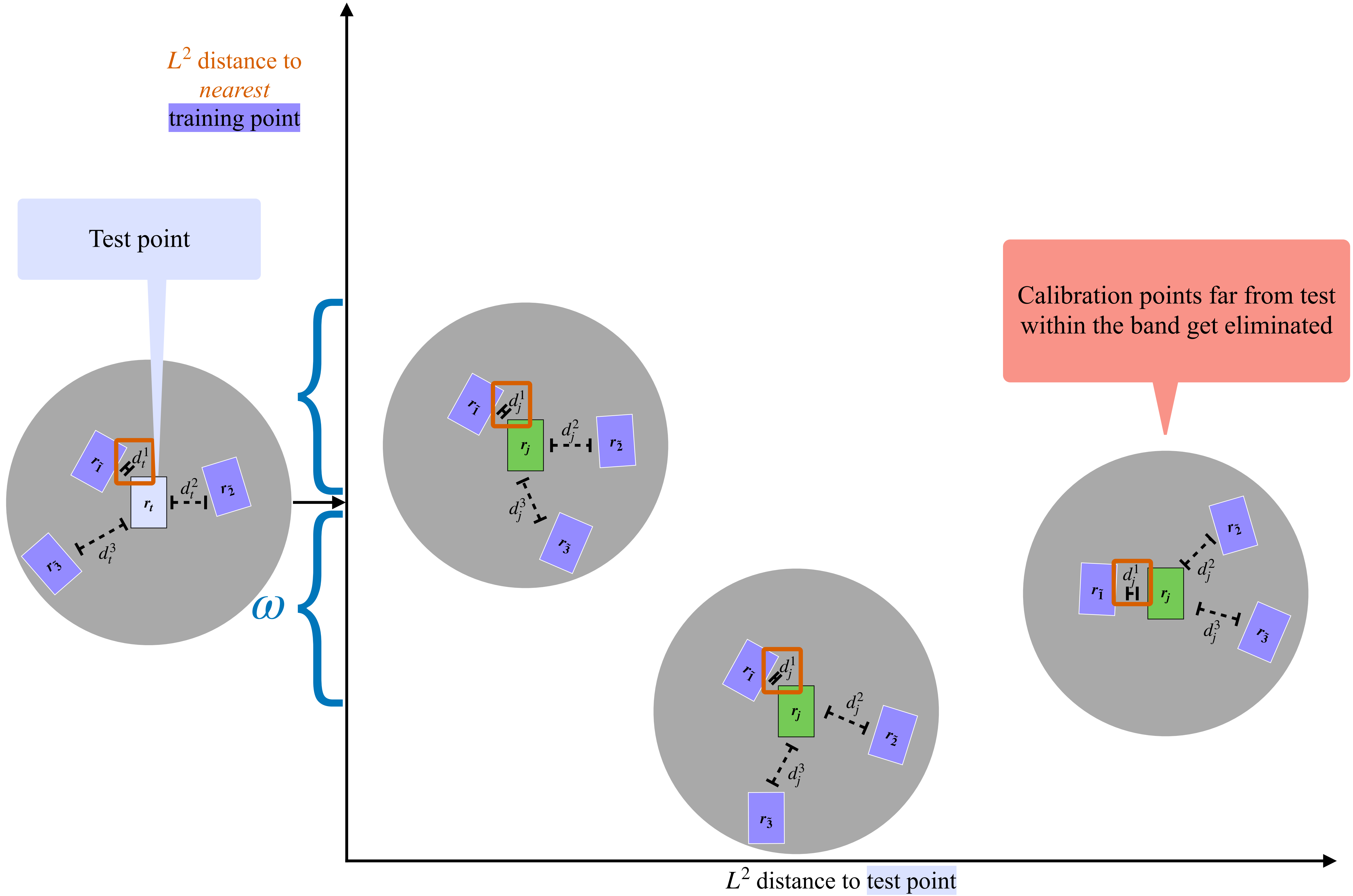

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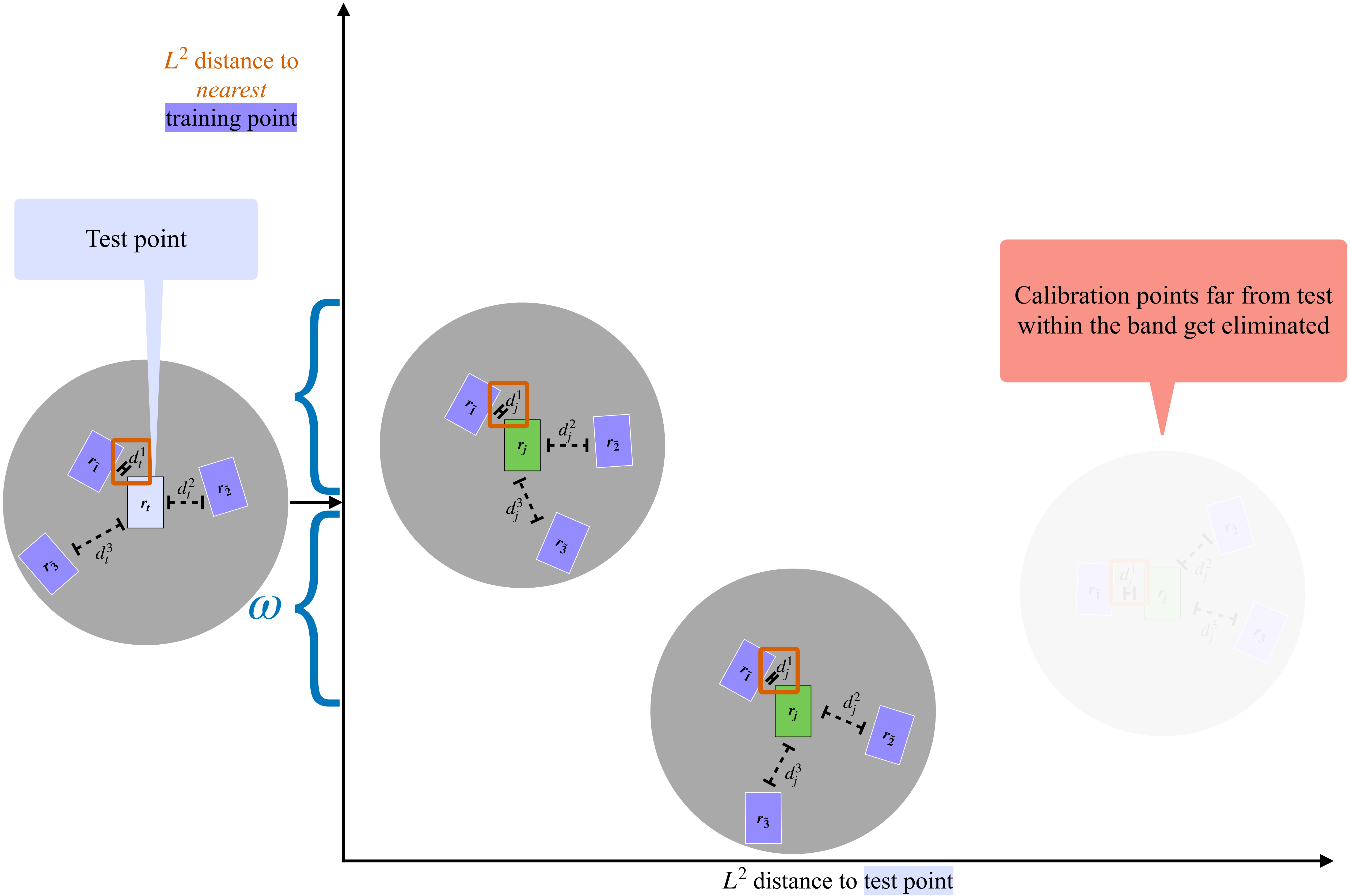

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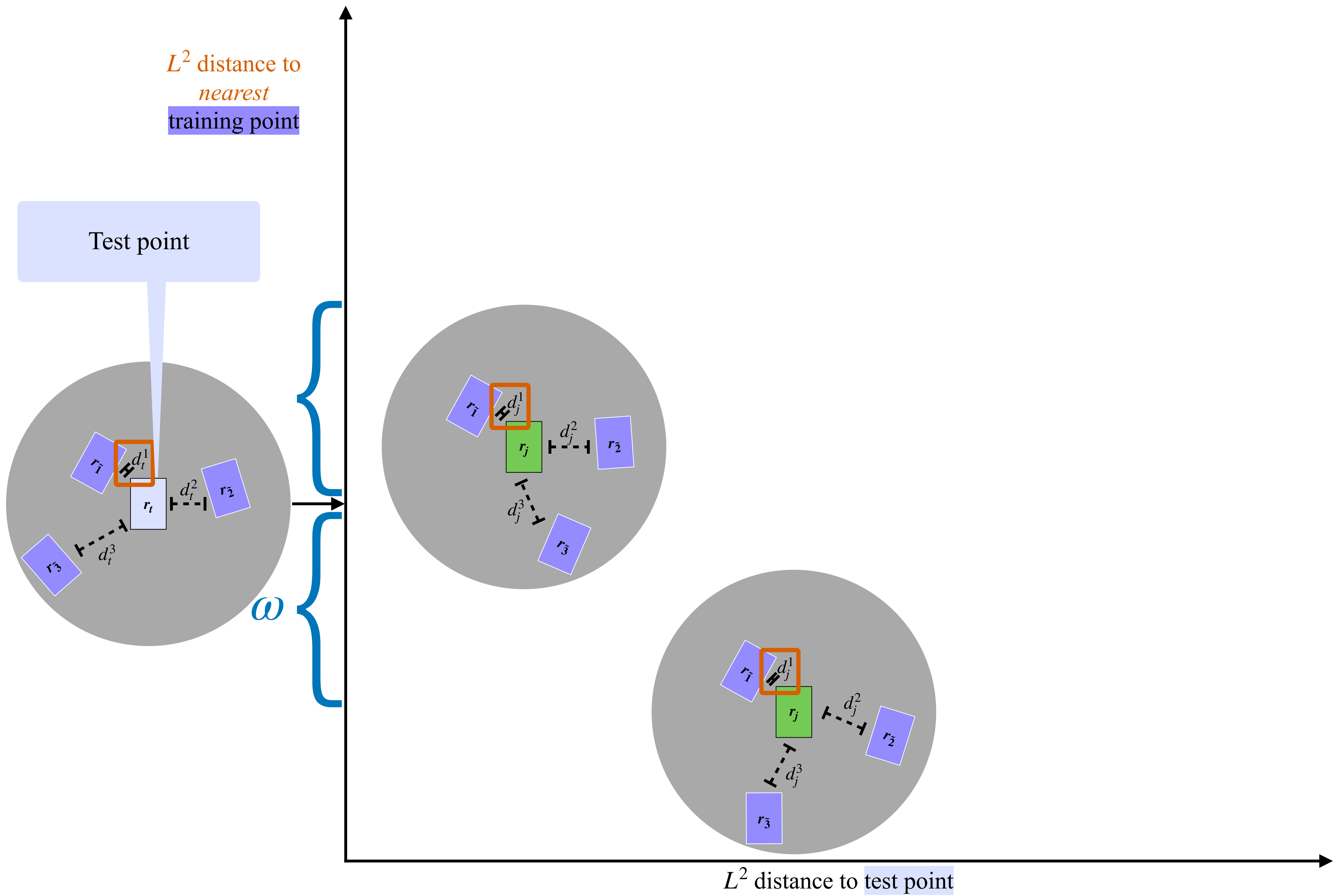
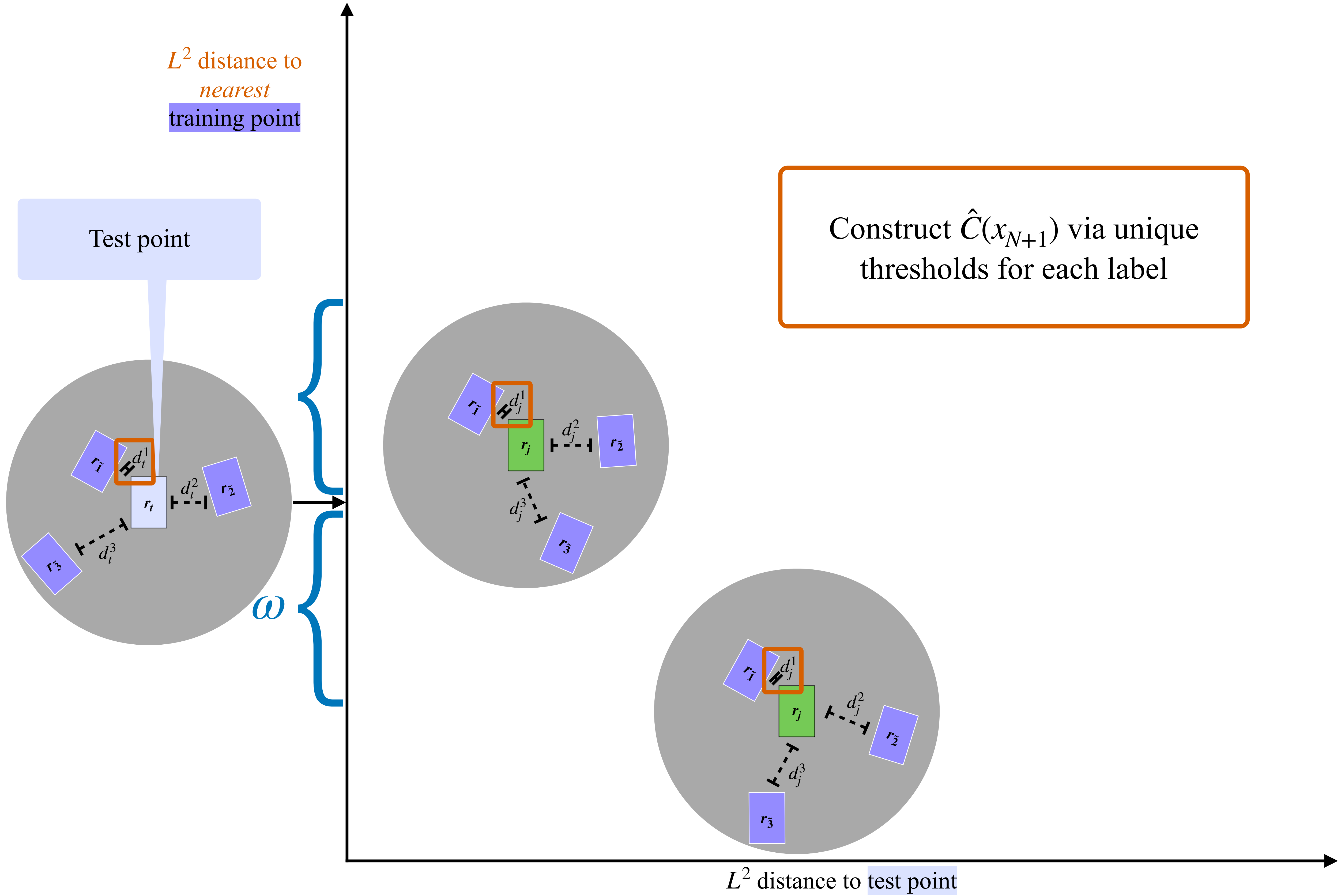
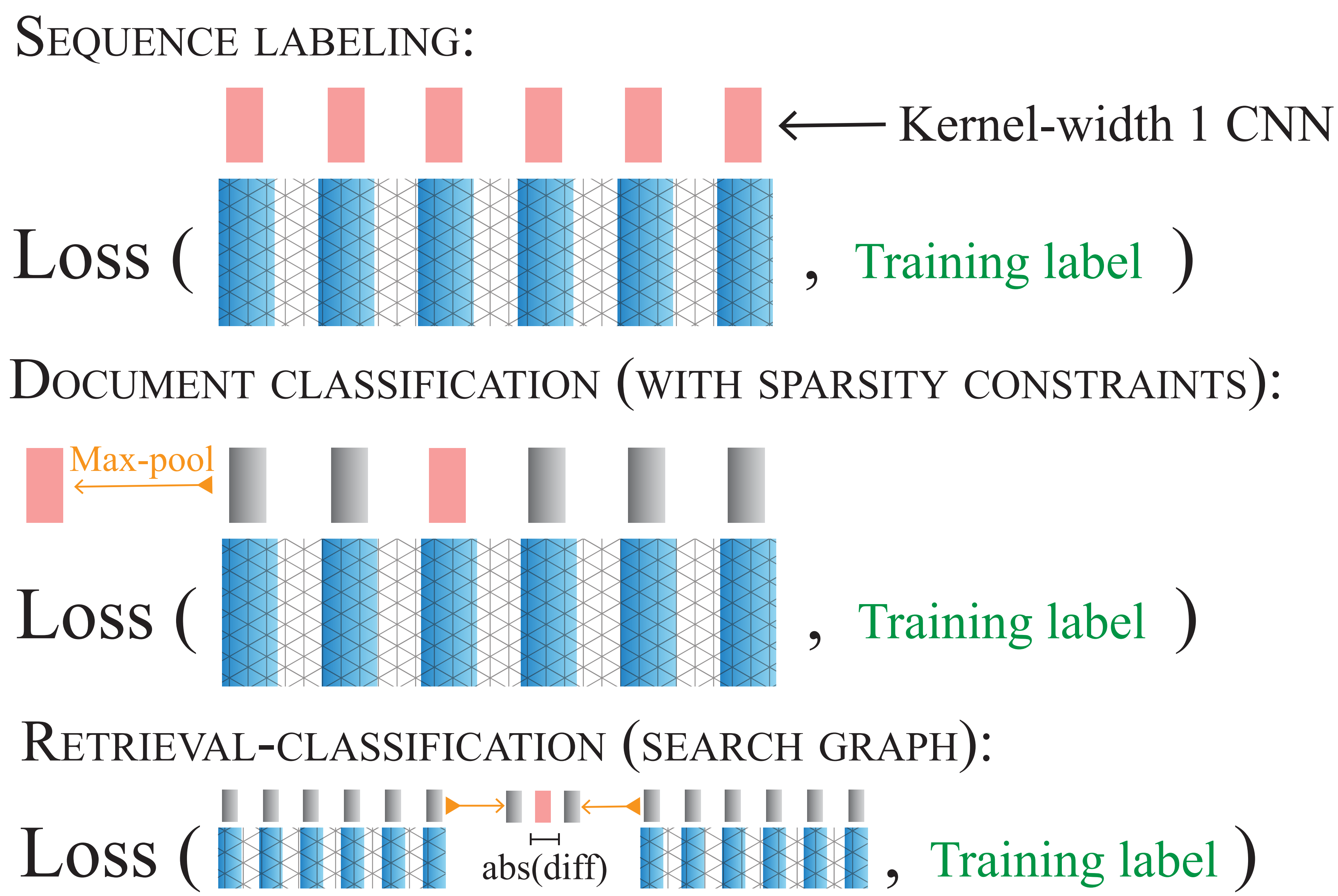


Label-conditional conformal thresholds



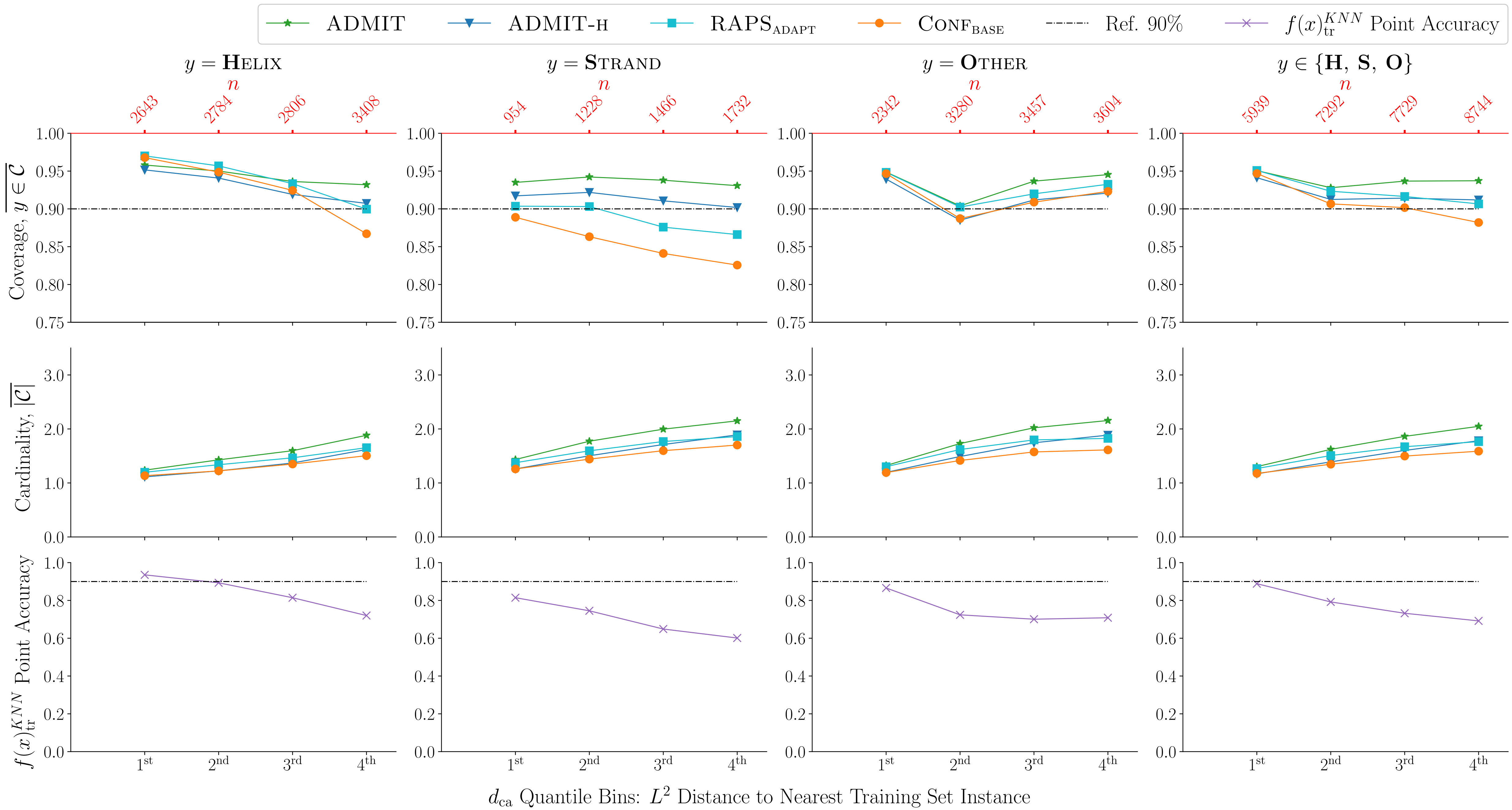
Construct $\hat{C}(x_{N+1})$ via unique thresholds for each label

Experiments



Task diversity: From in-distribution, high-accuracy *to* distribution-shifted, low-accuracy

Empirical behavior on in-domain data



Coverage, cardinality, and point accuracy for the TS115 test set from the PROTEIN task.

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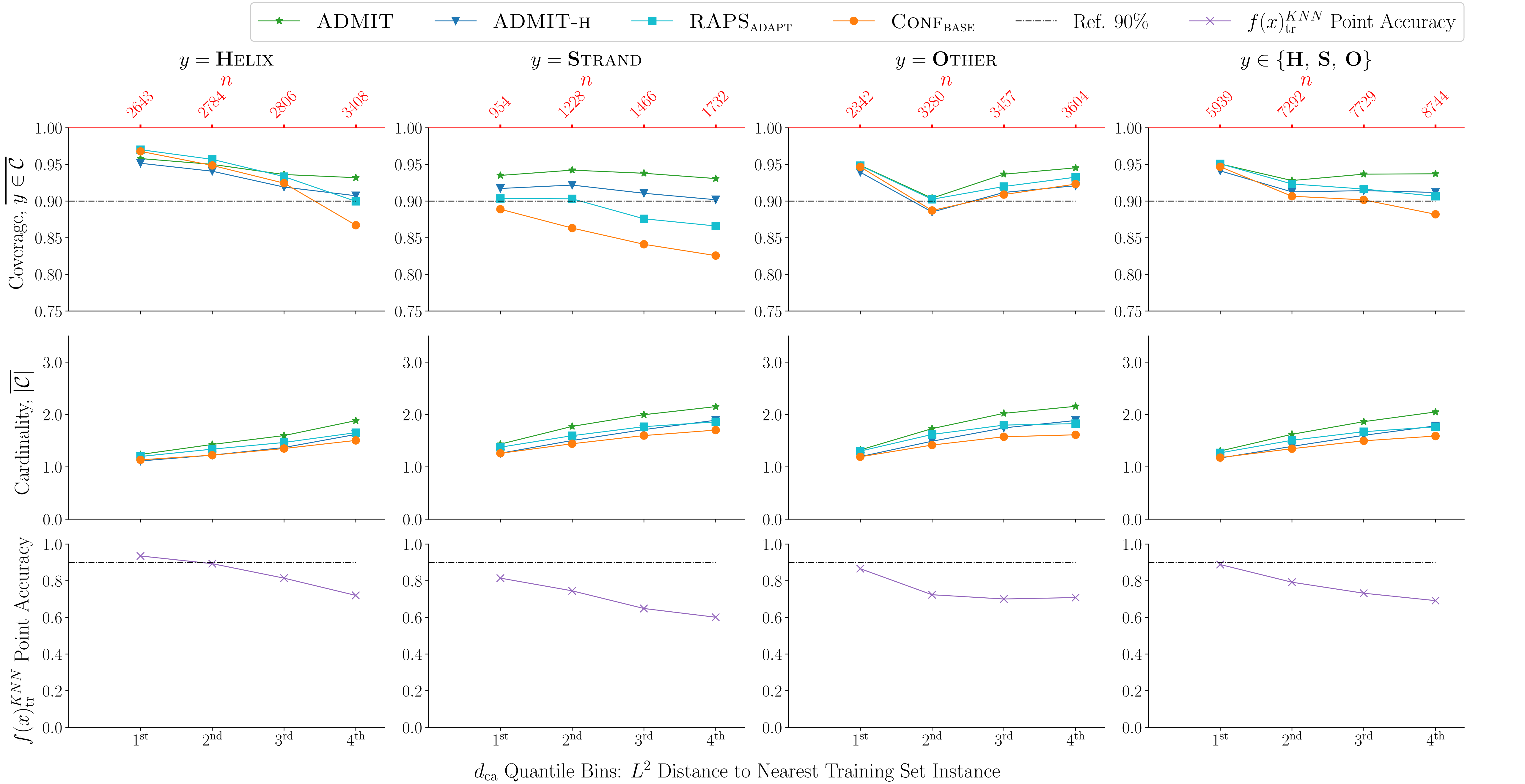

Coverage, cardinality, and point accuracy for the TS115 test set from the PROTEIN task.

Additional results

- Covariate/label shifts
- Heuristics for coverage conditioned on set composition
- And more …
- See: https://arxiv.org/abs/2205.14310

ADMIT: A general framework for constructing, constraining, and analyzing point predictions and distribution-free prediction sets for deep neural networks.