Isotonic Distributional Regression (IDR):
A powerful nonparametric calibration technique

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Introduction

**Goal:**
Provide calibrated probabilistic predictions for a real-valued quantity $Y$ (e.g. cumulated precipitation amount) based on an ensemble of predictions $X = (X^{(1)}, \ldots, X^{(d)})$.

**Requirement:**
Sufficient training data available: $(X_1, Y_1), \ldots, (X_n, Y_n)$

**Characteristics of IDR:**
- Generic (non-parametric) method providing a competitive benchmark for prediction (with respect to CRPS)
- Leads to calibrated probabilistic predictions (flat PIT histogram)
- (Almost) No tuning parameters
- May be outperformed by carefully tuned parametric postprocessing methods
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Fundamental assumption of IDR

“If the predictions increase we expect an increase of the outcomes.”
Making this intuition precise

“If the predictions increase. . .”

Partial order on the covariates:
\( x = (x_1, \ldots, x_d), x' = (x'_1, \ldots, x'_d) \in \mathbb{R}^d \)

\( x \preceq_p x' \) if \( x_1 \leq x'_1, \ldots, x_d \leq x'_d. \)

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Stochastic order on predictive distributions: \( F, G \) cdfs

\( F \preceq G \) if \( F(z) \geq G(z) \) for all \( z \in \mathbb{R}. \)

Equivalent:

\( F \preceq G \) if \( F^{-1}(\alpha) \leq G^{-1}(\alpha) \) for all \( \alpha \in (0, 1). \)
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Isotonic distributional regression (IDR)

Estimate the cdf-valued function $X \mapsto F_X$ with

$$F_X = \mathcal{L}(Y|X)$$

under the assumption that $F_X$ is isotone, that is,

$$X \leq_p X' \implies F_X \preceq F_{X'}.$$

**Minimization problem:** Define $\hat{F}_X$ to be the isotone cdf-valued $G_X$ minimizing

$$\frac{1}{n} \sum_{i=1}^{n} \text{CRPS}(G_{X_i}, Y_i).$$

**Result:** There exists a unique minimizer $\hat{F}_X$ which we call the IDR.
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Constructing the IDR

Let \( z \in \mathbb{R} \). Minimizing

\[
\sum_{\ell=1}^{n} (g_z(X_{\ell}) - \mathbb{1}\{Y_{\ell} > z\})^2
\]

everall increasing functions \( g_z : \mathbb{R}^d \rightarrow \mathbb{R} \) has a unique optimal solution that can be computed by solving a quadratic programming problem.

\[\hat{F}_X : z \mapsto 1 - \hat{g}_z(X) \text{ is a valid cdf}\]

\[X \mapsto \hat{F}_X \text{ is the IDR}\]

Sidenote:
Closed form of the optimal solution for a total order (\( d = 1 \))

\[
\hat{g}_z(X_{\ell}) = \min_{j \geq \ell} \max_{i \leq j} \frac{1}{(j - i + 1)} \sum_{t=i}^{j} \mathbb{1}\{Y_t > z\}.
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Optimality properties of the IDR

- Let $W$-CRPS be a quantile- or threshold-weighted CRPS. The IDR $\hat{F}_X$ satisfies

$$
\frac{1}{n} \sum_{\ell=1}^{n} W\text{-CRPS}(\hat{F}_{X_\ell}, Y_\ell) = \min_{G_X} \frac{1}{n} \sum_{\ell=1}^{n} W\text{-CRPS}(G_{X_\ell}, Y_\ell)
$$

where $G_X$ runs over all isotone cdf-valued functions.

- The IDR is calibrated “if the partial order is strong enough/the training sample is large enough”.

Using IDR for prediction

- Compute IDR for training dataset.
- For a new covariate value $X$, find nearest neighbors, choose suitable ones.
- Interpolate solution amongst nearest neighbors.
Application: Precipitation forecasts

Dataset

- Precipitation forecasts and observations from 2007 to 2017

<table>
<thead>
<tr>
<th>Airport</th>
<th>Available days (years)</th>
</tr>
</thead>
<tbody>
<tr>
<td>London Heathrow</td>
<td>2256 (6.2)</td>
</tr>
<tr>
<td>Brussels</td>
<td>3406 (9.4)</td>
</tr>
<tr>
<td>Zurich Kloten</td>
<td>3241 (8.9)</td>
</tr>
<tr>
<td>Frankfurt</td>
<td>3617 (9.9)</td>
</tr>
</tbody>
</table>

- Observations: 24-hour accumulated precipitation amounts
- Forecasts: ECMWF ensemble
  52 members: high-resolution forecast (HRES), control forecast (CTRL), 50 perturbed members (PM)
- IDR using (HRES, CTRL, mean of PM)
Results: CRPSS

CRPS skill score (relative to ENS)

Frankfurt
Zurich
London
Brussels
Discussion and outlook

- IDR is a new generic technique to generate calibrated probabilistic predictions.
- IDR can accommodate predictions from multiple models.
- IDR is in-sample optimal with respect to all weighted CRPS.
- IDR provides guarantees for calibration in-sample.
- IDR yields competitive predictions for precipitation using less information.
- R Package for IDR in preparation

Extensions/related methods:

- Semi-parametric IDR for outcomes with heavy tails.
- Isotonic regression for point predictions/specific parameters of the predictive distribution.