# On the generation of probabilistic forecasts from deterministic models

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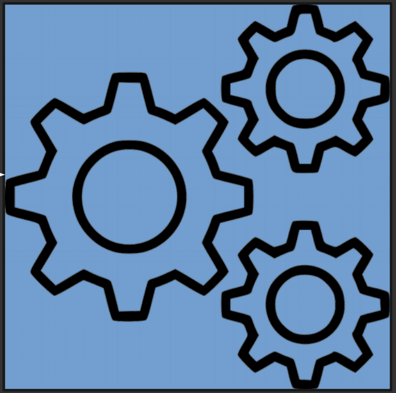
Jacob Bortnik (UCLA), Algo Care' (U. Brescia, Italy)

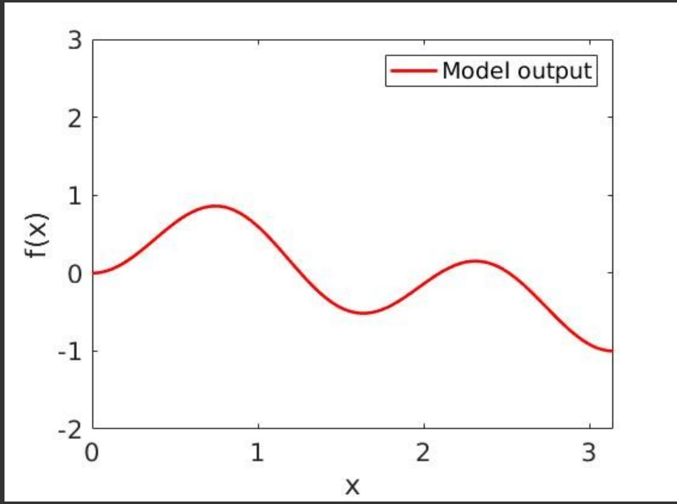
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 776262 (AIDA)

# Problem statement

Set of Inputs,
Parameters,
etc.



Deterministic model



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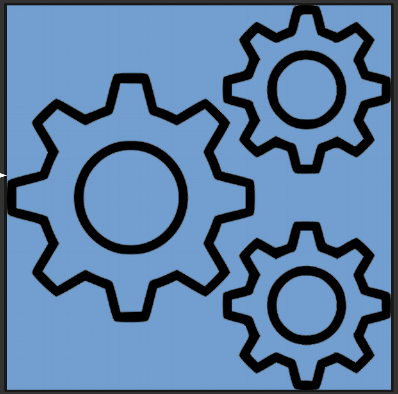
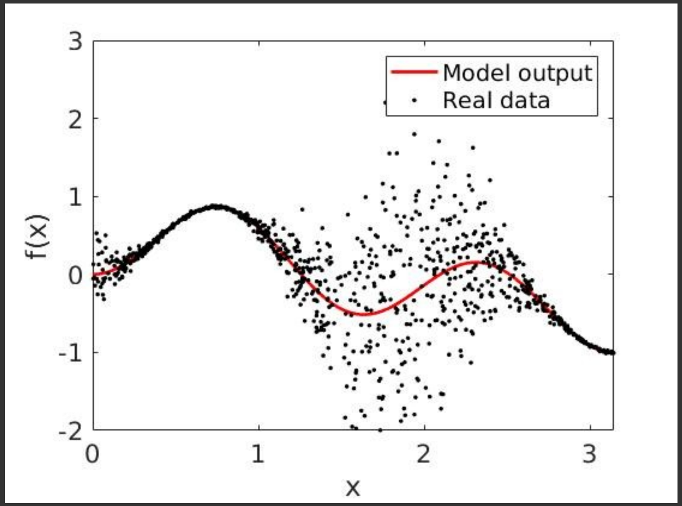


Deterministic model + Real Data




Uncertainties:

- Epistemic (do not know the parameters exactly)
- Aleatoric (physics that is not in the model)
- Algorithmic (numerical errors)

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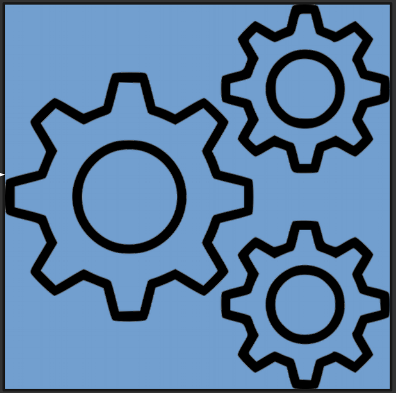

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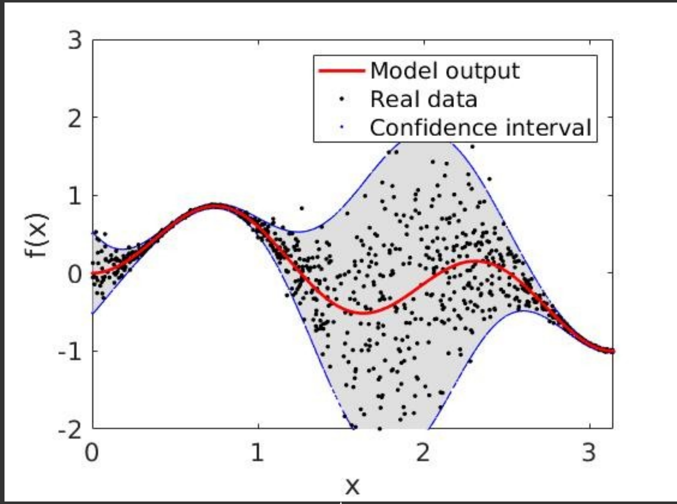


Uncertainties:

- Epistemic (do not know the parameters exactly)
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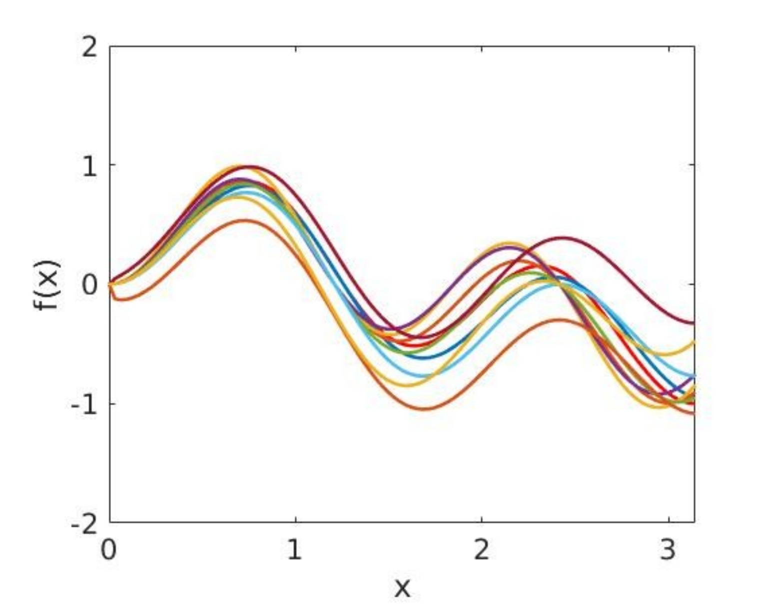
?

Generate heteroskedastic uncertainty

# Standard Approach

- The golden standard approach to estimate uncertainties based on a deterministic model is by running a

  **Monte Carlo ensemble**
  (e.g. by small perturbations of initial conditions)

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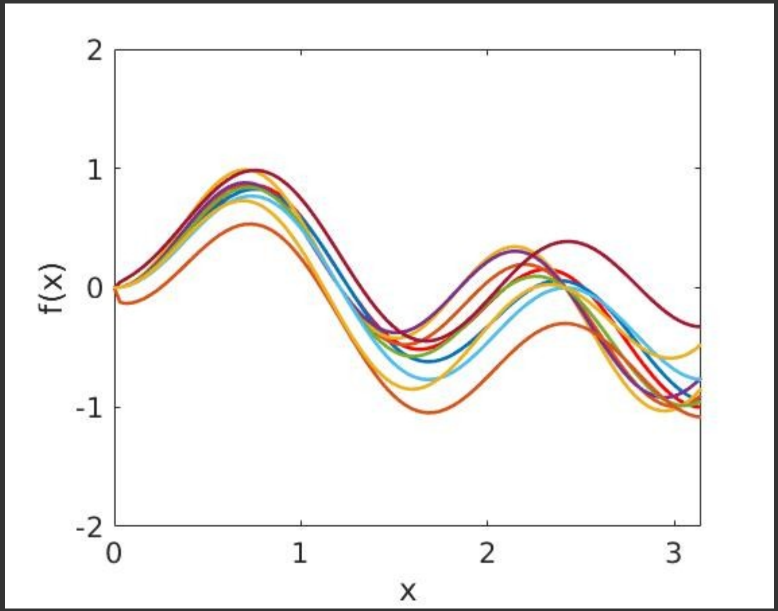


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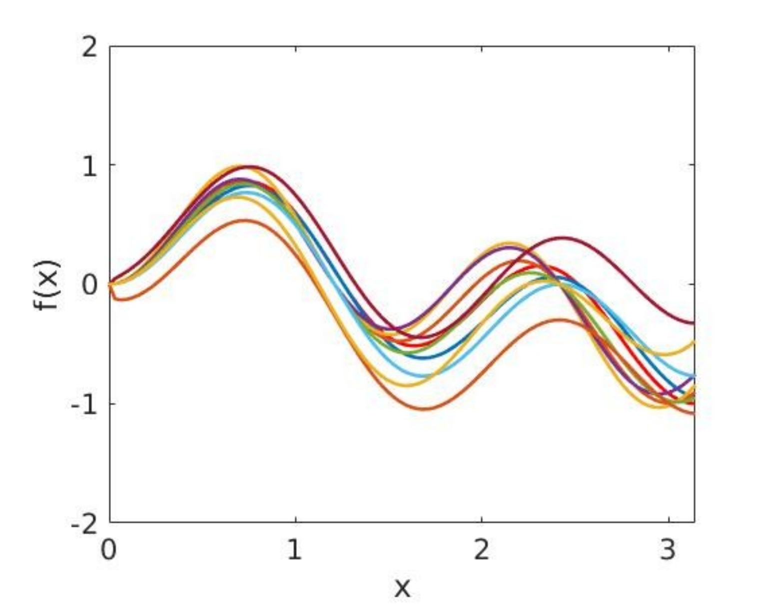



- This has two problems:
  - It requires many runs (expensive)
  - It requires to know what is the probability distribution of inputs
    (as in the work of R. Sarma , Thursday morning)

# Take home message

We have devised a method that:

- Estimates the uncertainties associated with single-point outputs generated by a deterministic model, in terms of Gaussian distributions;
- Ensures the optimal trade-off between accuracy and reliability;
- Does not need to run ensembles. It costs as much as training a neural network
- Code available: zenodo.1485608

Space Weather

RESEARCH ARTICLE

10.1029/2018SW002026

**Key Points:**

- We introduce a new method to estimate the uncertainties associated with single-point outputs generated by a deterministic model
- The method ensures a trade-off between accuracy and reliability of the generated probabilistic forecasts
- Computationally cheap model:

## On the Generation of Probabilistic Forecasts From Deterministic Models

E. Camporeale[1,2], X. Chu[3], O. V. Agapitov[4], and J. Bortnik[5]

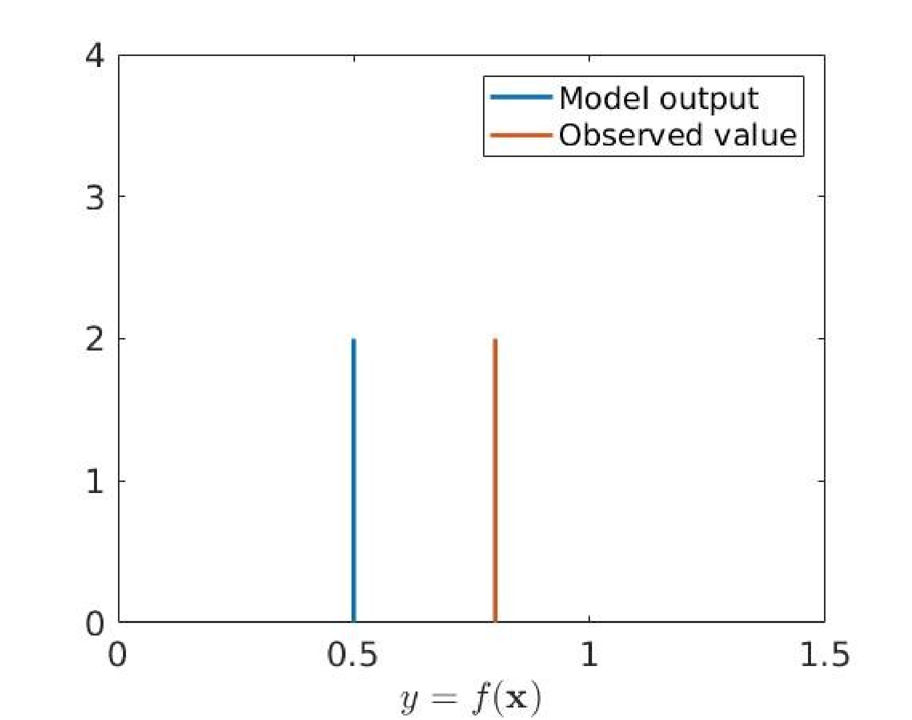
[1]Center for Mathematics and Computer Science (CWI), Amsterdam, The Netherlands, [2]Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, CO, USA, [3]Laboratory for Atmospheric and Space Physics, University of Colorado, Boulder, CO, USA, [4]Space Sciences Laboratory, University of California Berkeley, Berkeley, CA, USA, [5]Department of Atmospheric and Oceanic Sciences, University of California, Los Angeles, CA, USA

# Utilitarian Approach

Let us assume that for a single (multidimensional) input **x**, our model predicts an output y = f(x).

Blue line → Model output
Red line → Real (observed value)

Working hypothesis:
We want to use the model output as the mean of a Gaussian distribution that is interpreted as a probabilistic forecast.



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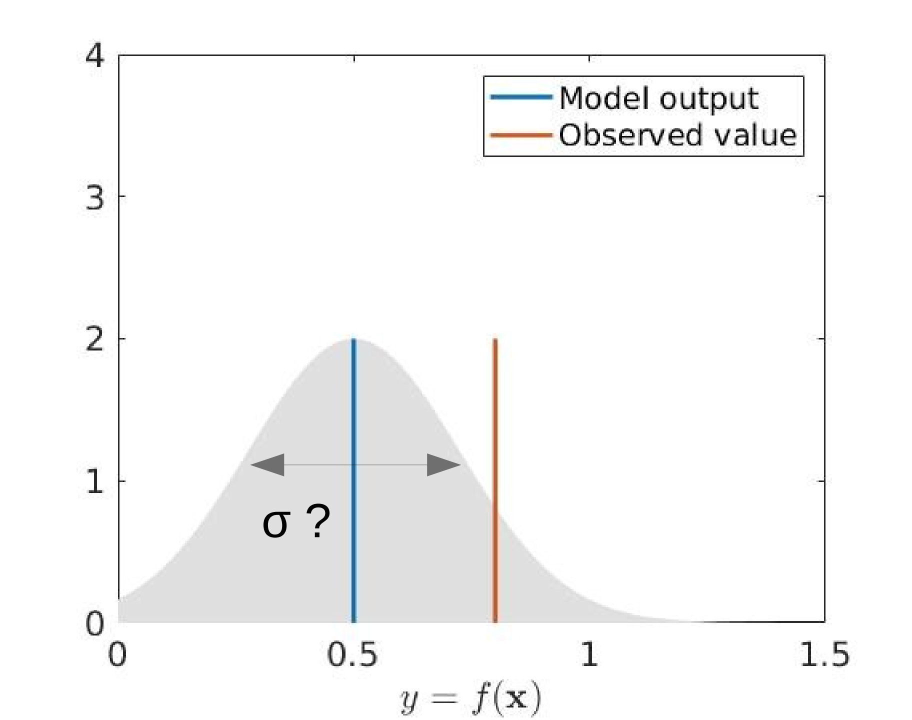
**What is the optimal width of a Gaussian forecast?**



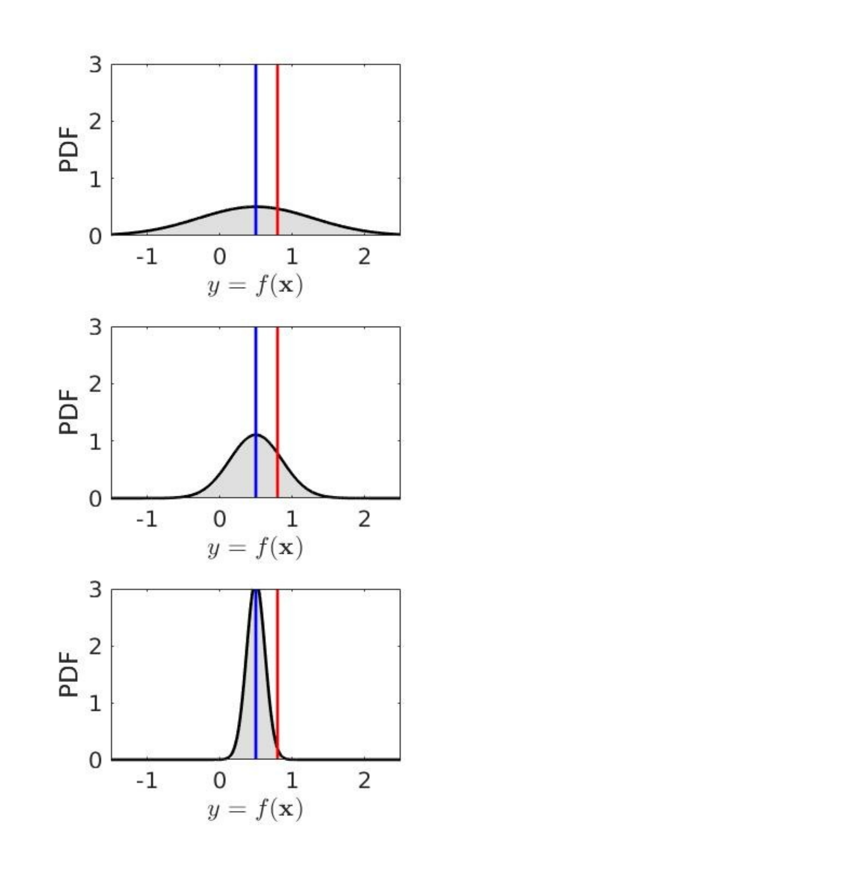
# Continuous Rank Probability Score

What is the optimal width of a Gaussian forecast?

"Optimal" with respect to what?

We use the CRPS as a score for "accuracy".

- CRPS is a generalization of Brier score
- It has a simple graphical interpretation
- CRPS = 0 for perfect forecast

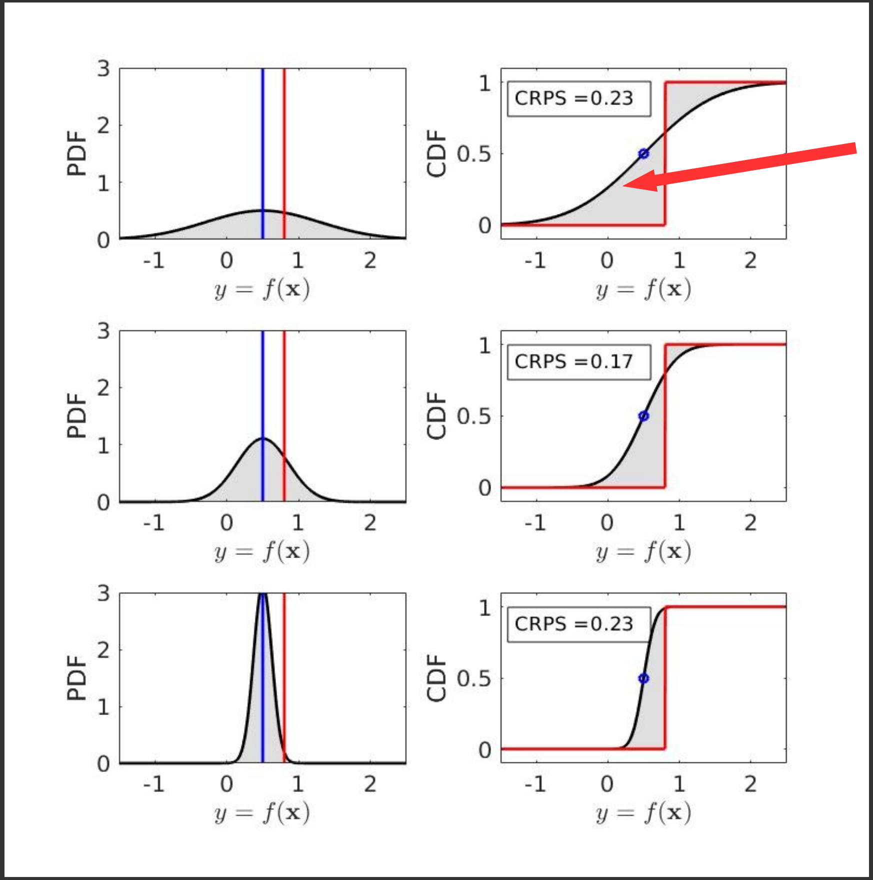


# Continuous Rank Probability Score

- CRPS is a generalization of Brier score
- It has a simple graphical interpretation
- CRPS = 0 for perfect forecast
- CRPS = $\int \left( C(y) - H(\hat{y}) \right)^2 dy$

CDF

Step function




CRPS proportional to this area

# Continuous Rank Probability Score

For a Gaussian distribution, CRPS has an analytical expression which is a function of:

- Error ε: difference between model output and observed value
- Standard deviation σ

If we define the optimal σ the one that minimizes CRPS

we obtain a probabilistic forecast that is not RELIABLE

# What is a probabilistic forecast anyway?

*Risk Analysis, Vol. 25, No. 3, 2005*

DOI: 10.1111/j.1539-6924.2005.00608.x

**"A 30% Chance of Rain Tomorrow": How Does the Public Understand Probabilistic Weather Forecasts?**

**Gerd Gigerenzer,[1]* Ralph Hertwig,[2] Eva van den Broek,[1] Barbara Fasolo,[1] and Konstantinos V. Katsikopoulos[1]**

TABLE 2. Responses to Q14a, the meaning of the forecast "There is a 60% chance of rain for tomorrow" ($N$ = 1330).

| | Percent of respondents |
|---|---|
| It will rain tomorrow in 60% of the region. | 16 |
| It will rain tomorrow for 60% of the time. | 10 |
| It will rain on 60% of the days like tomorrow.* | 19 |
| 60% of weather forecasters believe that it will rain tomorrow. | 22 |
| I don't know. | 9 |
| Other (please explain). | 24 |

* Technically correct interpretation, according to how PoP forecasts are verified, as interpreted by Gigerenzer et al. (2005).

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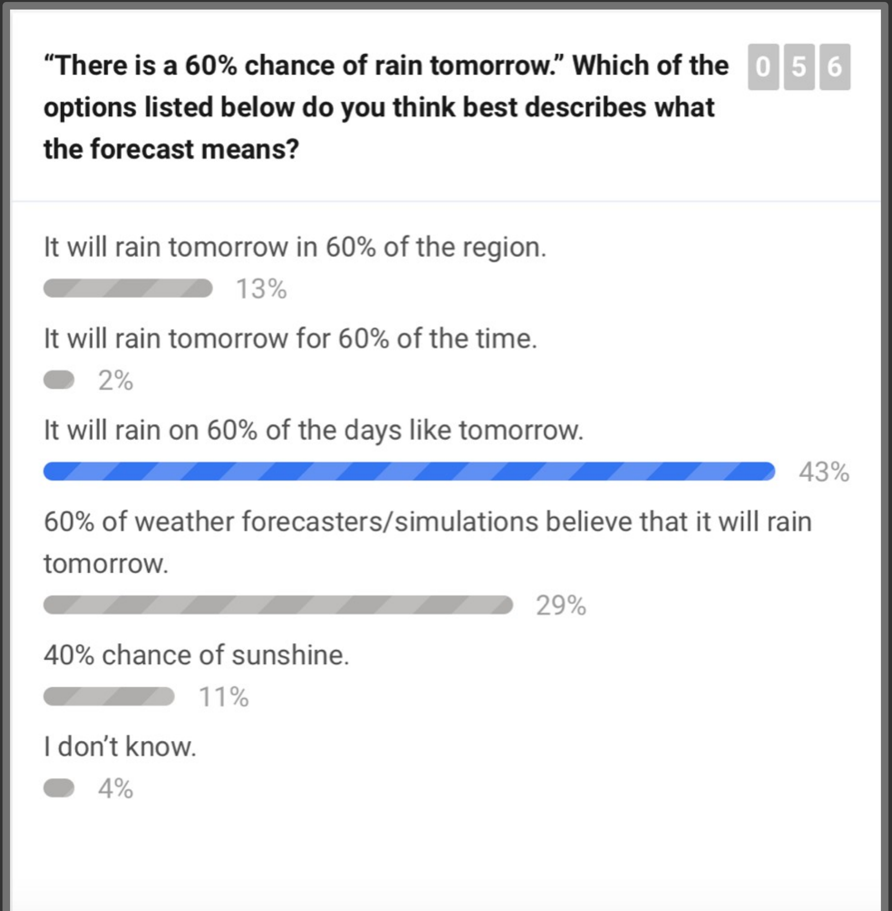
**Communicating Uncertainty in Weather Forecasts: A Survey of the U.S. Public**

REBECCA E. MORSS, JULIE L. DEMUTH, AND JEFFREY K. LAZO

*National Center for Atmospheric Research,* Boulder, Colorado*

# What is a probabilistic forecast anyway?

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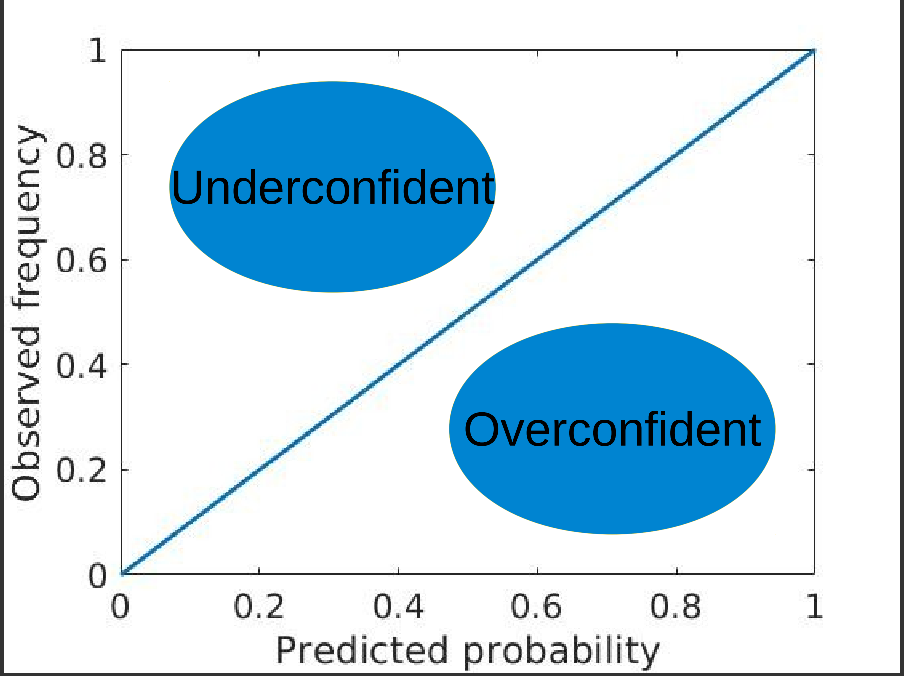
# Reliability diagram

Reliability is the property of a probabilistic model that measures its **statistical consistency with observations.**

For example, for forecasts of discrete events, the reliability measures if an event occurs on average with frequency *p*, when it has been predicted to occur with probability *p*.



# Reliability diagram

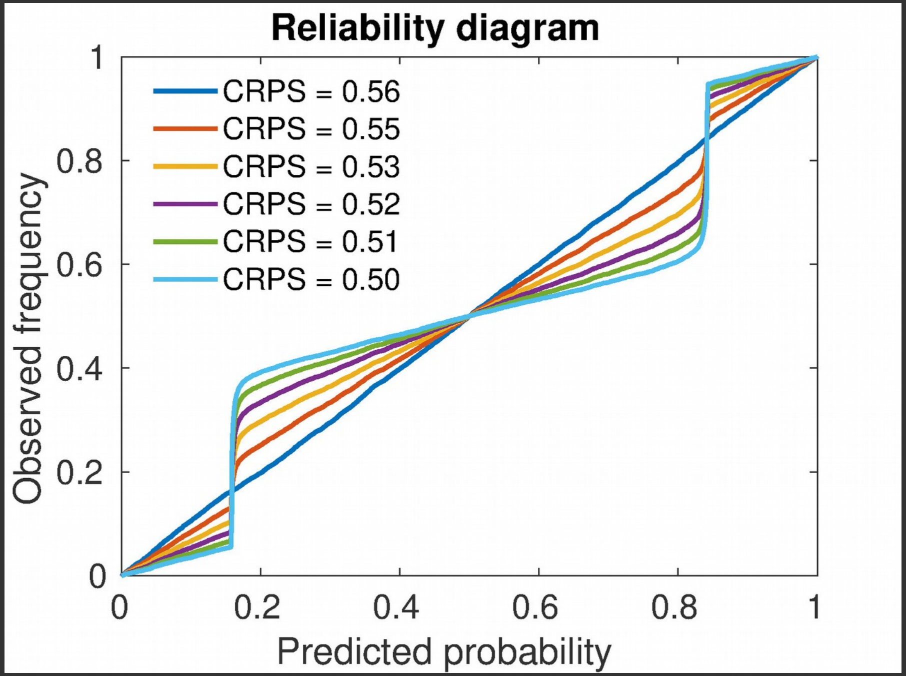
The values of σ that minimize CRPS can be derived analytically:

$$\sigma^2_{opt} \sim \varepsilon^2$$

The more we minimize CRPS, the worse reliability we get.

Mathematical proof is straightforward.

See arXiv:1811.12692



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The values of σ that minimize CRPS can be derived analytically:

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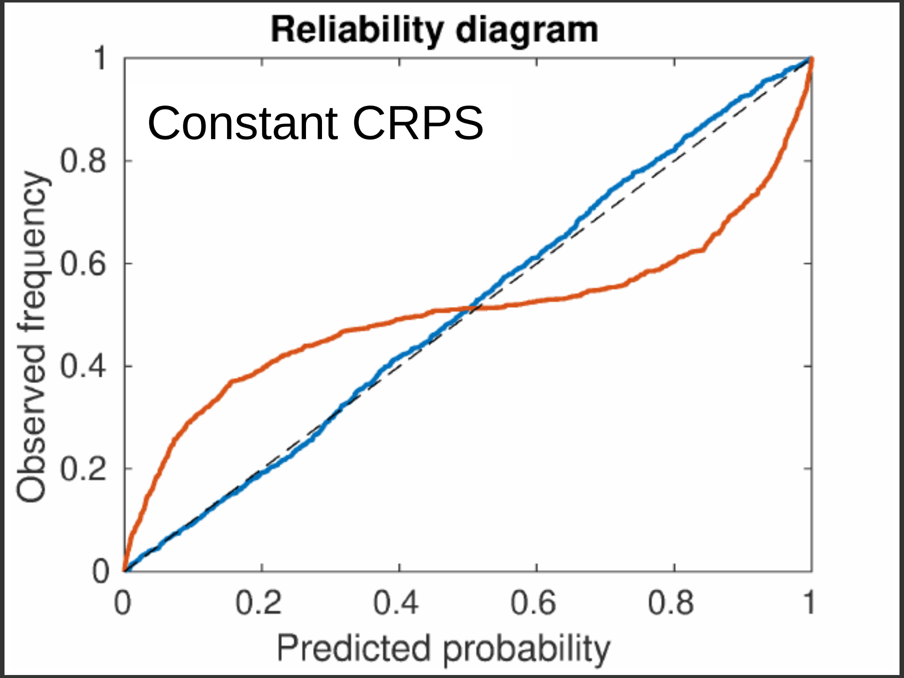
A given value of CRPS is not informative on the reliability

See arXiv:1811.12692



# Reliability Score

We define an analytical Reliability Score (RS)

- It measures how far the distribution of standardized errors ε/σ is from a Standard Normal distribution (other definition of reliability)

$$\eta_i = \varepsilon_i/(\sqrt{2}\sigma_i), \tag{5}$$

where the standard deviations $\sigma_i$ are determined by the input vector. If $\sigma(\mathbf{x})$ is not constant then this definition acts to both standardize and transform the error distribution. While the forecast errors $\varepsilon_i$ may not be Gaussian, in the case of a normally distributed forecast we expect $\eta$ calculated over a sample of N prediction-observation pairs to follow a standard normal distribution with CDF $\Phi(\eta) = \frac{1}{2}(\mathrm{erf}(\eta)+1)$. Hence, we define the Reliability Score (RS) as

$$\mathrm{RS} = \int_{-\infty}^{\infty} \left[\Phi(y) - C_\eta(y)\right]^2 dy, \tag{6}$$

where $C_\eta(y)$ is the empirical cumulative distribution of the standardized errors $\eta$, that is

$$C_\eta(y) = \frac{1}{N}\sum_{i=1}^{N} H(y - \eta_i) \tag{7}$$

with $\eta_i = (y_i^o - \mu_i)/(\sqrt{2}\sigma_i)$.

# Two-objective cost function

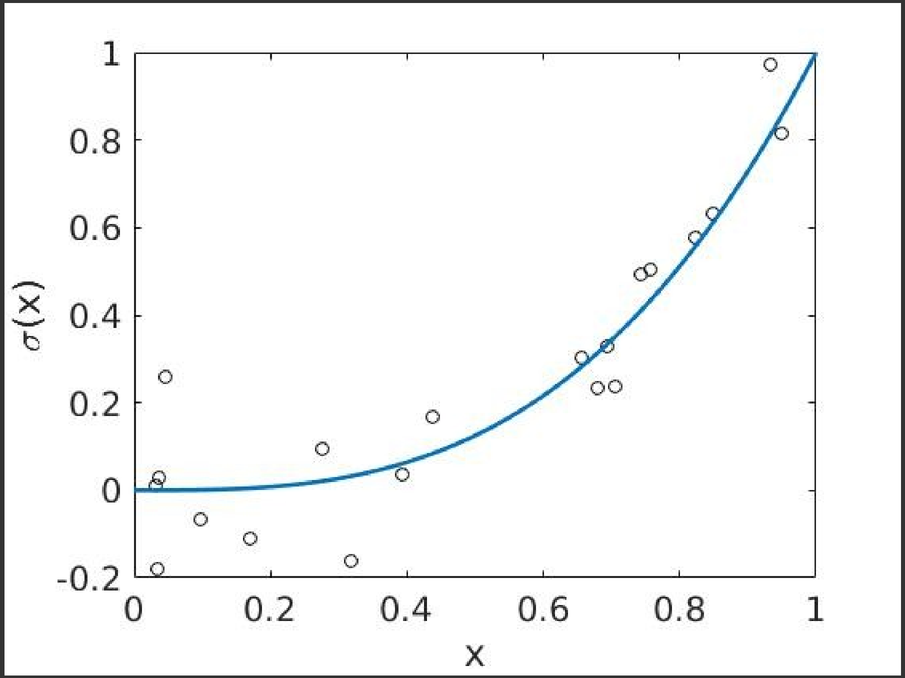
- This is a two-objective optimization problem, because reliability and accuracy are competing objectives.
- We define the Accuracy-Reliability (AR) cost function:

$$AR = \underbrace{CRPS}_{\text{Accuracy}} + \beta * \underbrace{RS}_{\text{Reliability}}$$

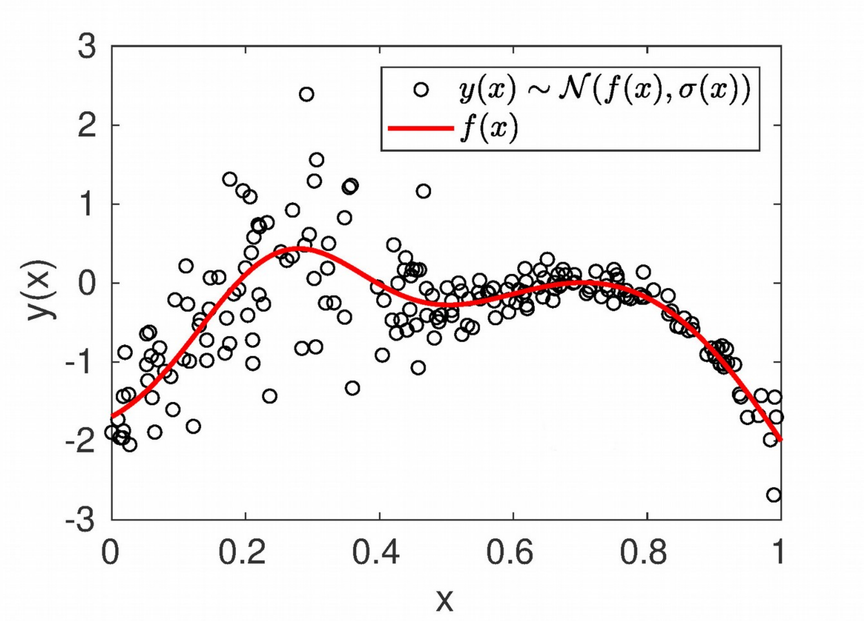
- Accuracy and Reliability cannot both be minimized simultaneously
- We have to find the best trade-off

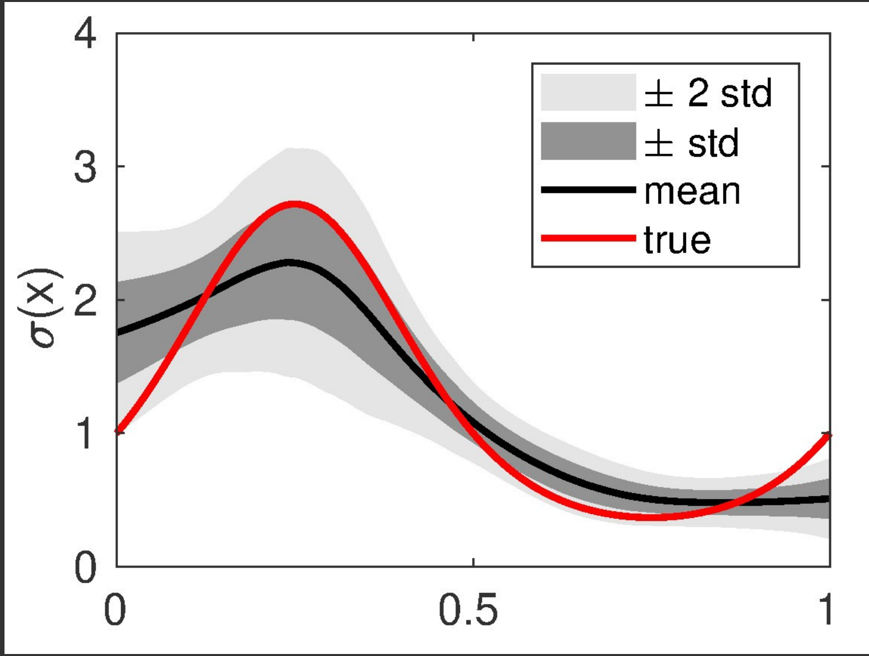
# The Method

- Take a sample of N errors ε (difference between model output and observed values) and the corresponding model inputs **x**
- We define as optimal standard deviation σ the one that optimizes the Accuracy-Reliability cost function (that has an analytical expression)
- We also want to have a way of generating a smooth function σ(**x**) for any value of **x**
- We use a neural network that takes **x** as input and produces σ(**x**) as output by minimizing AR cost function.



# Synthetic example



# DEN2D: model for plasmasphere electron density

Estimates the electron density based on history of geomagnetic indexes using a Neural Network.

X. Chu et al. *JGR* (2017)

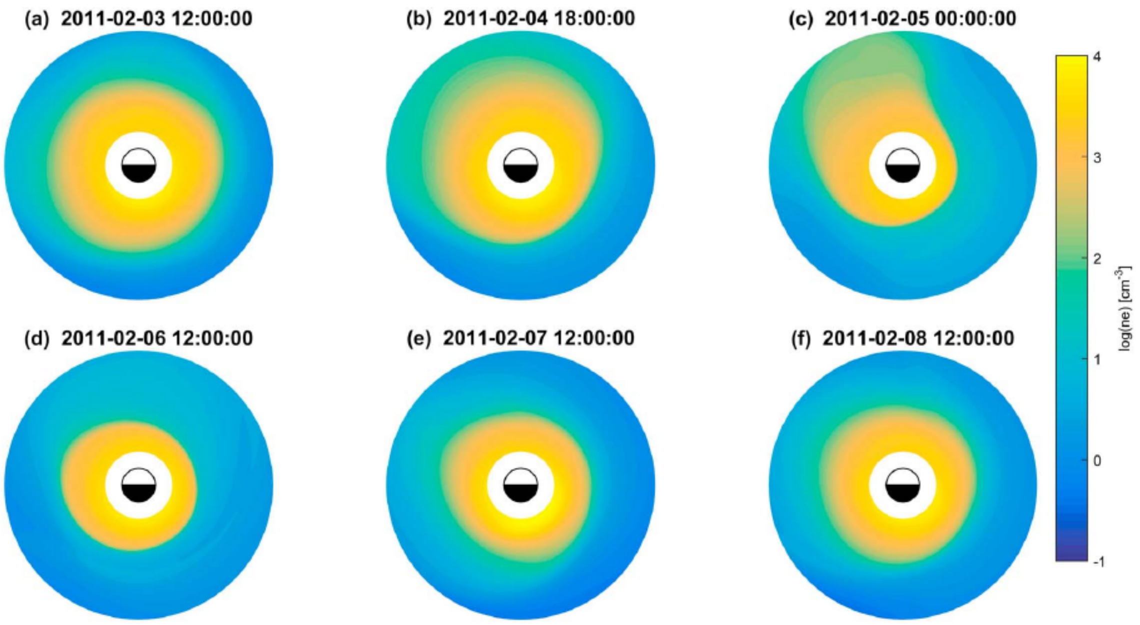



**Figure 6.** A series of panels showing the neural network reconstruction of the global plasma density in the equatorial plane as a function of *L* and MLT at the following times: (a) 2011–02-03/12:00:00 (quiet time before the storm); (b) 2011–02-04/18:00:00 (during the main phase); (c) 2011–02-05/00:00:00 (at the minimum of *SYM-H*); (d) 2011–02-06/12:00:00, (e) 2011–02-07/12:00:00, and (f) 2011–02-08/12:00:00 (recovery phase). The colorbar represents the logarithm of the electron number density in el/cc.

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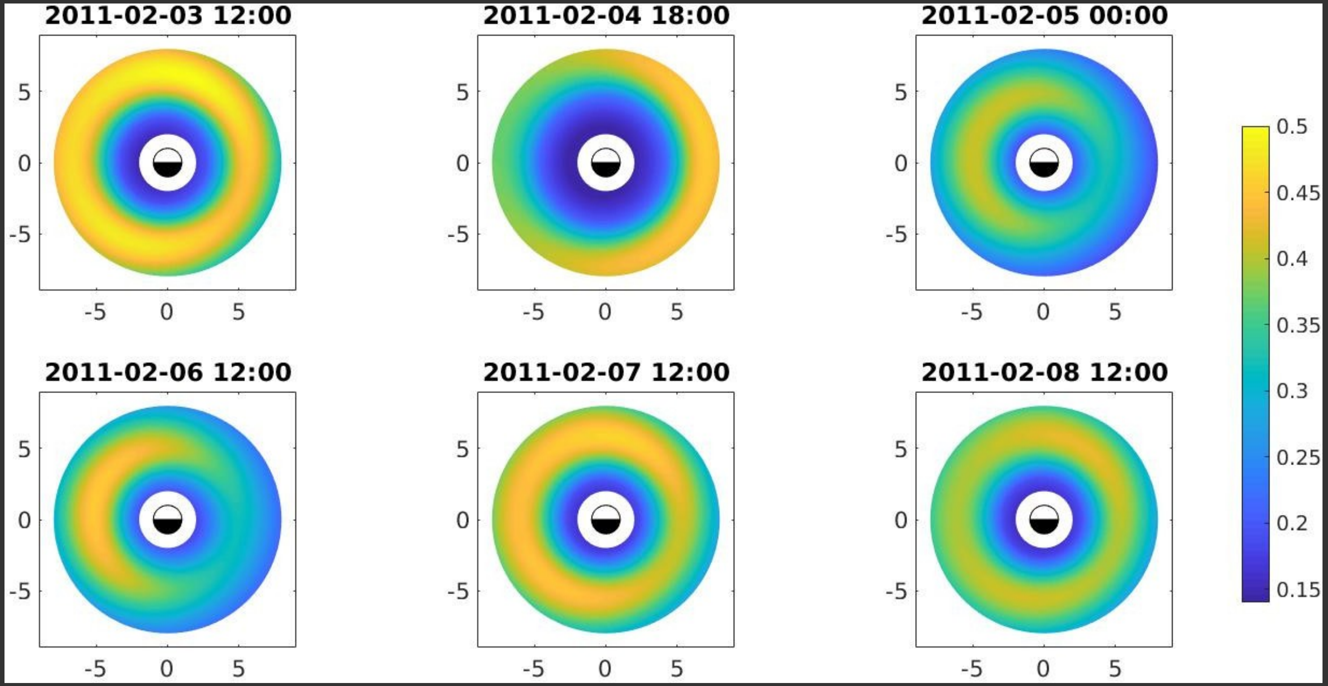


Estimate of the standard deviation (uncertainty) with the AR method

# Machine Learning benchmark

Table 1: Comparison between different methods on several multidimensional dataset.

| Method | | | NLPD | KM | RECAL | AR | NLPD | KM | RECAL | AR | NLPD | KM | RECAL | AR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Score | | | NLPD | | | | CRPS | | | | Cal. err. (%) | | | |
| Dataset | Size | Dim. | | | | | | | | | | | | |
| Boston Housing | 506 | 13 | 0.64 | 1.42 | **0.52** | 0.90 | 0.27 | 0.54 | **0.25** | 0.83 | 10.5 | 8.7 | 14.4 | **8.3** |
| Concrete | 1,030 | 8 | 0.55 | 0.84 | **0.50** | 0.62 | 0.26 | 0.28 | **0.22** | 0.26 | 6.0 | 19.7 | 10.6 | **5.3** |
| Energy | 768 | 8 | -0.31 | -0.30 | **-0.12** | -0.23 | 0.13 | **0.08** | 0.14 | 0.13 | 9.6 | 28.4 | 15.6 | **7.7** |
| Kin8nm | 8,192 | 8 | 0.32 | 0.85 | 0.57 | **0.31** | **0.2** | 0.24 | 0.24 | **0.2** | 2.8 | 24.7 | 6.7 | **2.0** |
| Naval propulsion | 11,934 | 15 | -1.52 | 0.84 | -0.82 | **-1.58** | 0.06 | 0.22 | **0.05** | 0.06 | 6.6 | 45 | **2.0** | 4.4 |
| Power plant | 9,568 | 4 | **0.04** | 0.25 | 0.28 | **0.04** | 0.15 | 0.15 | 0.15 | 0.15 | 3.1 | 15.8 | **2.6** | **2.6** |
| Protein | 45,730 | 9 | **1.11** | 1.18 | 1.18 | 1.18 | 0.43 | 0.43 | 0.45 | **0.42** | 7.4 | 8.3 | **1.0** | 7.4 |
| Wine | 1,599 | 11 | 1.24 | **1.16** | 1.20 | 1.29 | 0.47 | **0.43** | 0.46 | 0.47 | 11.9 | 11.3 | **5.5** | 10.6 |
| Yacht | 308 | 6 | -0.44 | 0.39 | **-0.64** | -0.25 | 0.12 | 0.20 | **0.09** | 0.12 | 16.2 | 27.8 | 20.4 | **12.0** |

Lesson learned from ML community: new methods are always tested against standard benchmarks and compared with ‘baseline’ methods

# Take home message

We have devised a method that:

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