Hello! 👋

Sam Hunt **Pieter De Vis**

Mentimeter Survey

Code: 1687 1279

Workshop Materials

IDEAS-QA4EO

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Today's Agenda

1. **Presentation: CoMet Toolkit Introduction**
   - ❑ *What is CoMet?*
   - ❑ *Uncertainty 101*
   - ❑ *Tools Intro*
2. **Exercises**
   - ❑ **punpy** basics with in-situ type data
   - ❑ **obsarray** basics with EO type data
3. **"Real-life" Examples**

Workshop Materials

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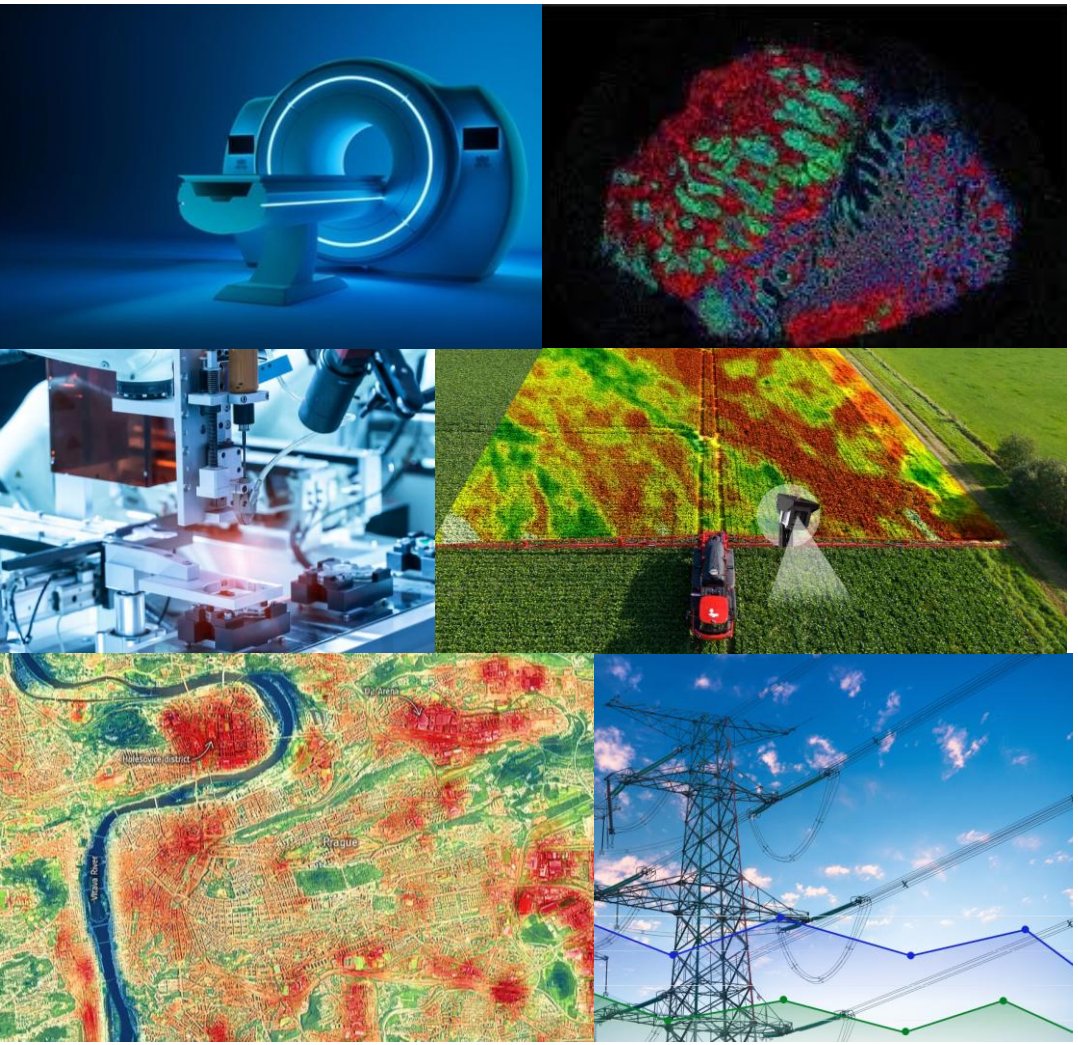
The CoMet Toolkit – Uncertainties made easy

Sam Hunt, Pieter De Vis, Maddie Stedman
National Physical Laboratory

Imperial College London hands-on tutorial - 19/03/2025

Measurements in Society



- Critical for e.g. **health**, **manufacturing**, and **environmental** monitoring.
- Growing in **size** and **complexity**.
- Reliable interpretation requires **uncertainty and error-covariance** information, often overlooked or non-standardised.
- **Error correlation** important to get uncertainties right when combining data

NPL

What is National Physical Laboratory?

- UK's **National Metrology Institute** (NMI)
- "Realises, maintains and develops the UK's primary measurement standards"
- Established in 1900

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CoMet Toolkit

Python Tools

Uncertainty Handling

Open Source

Tested

Applied

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CoMet Toolkit

punpy

Propagation UNcertainties in Python

obsarray

Handling uncertainty and error-covariance in datasets

comet_maths

CoMet mathematical algorithms and interpolation tools

UNC Specification

Uncertainty metadata naming conventions

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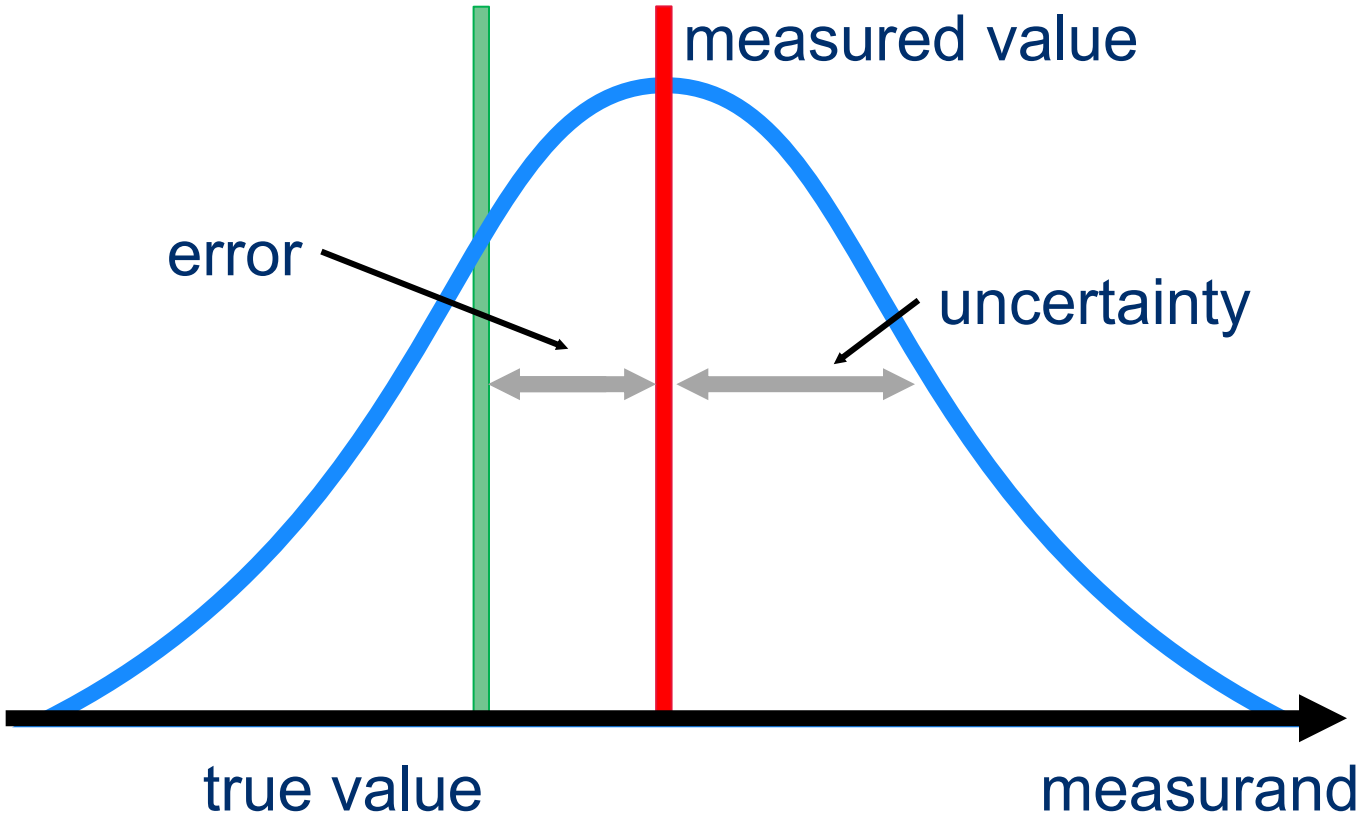
Uncertainties 101



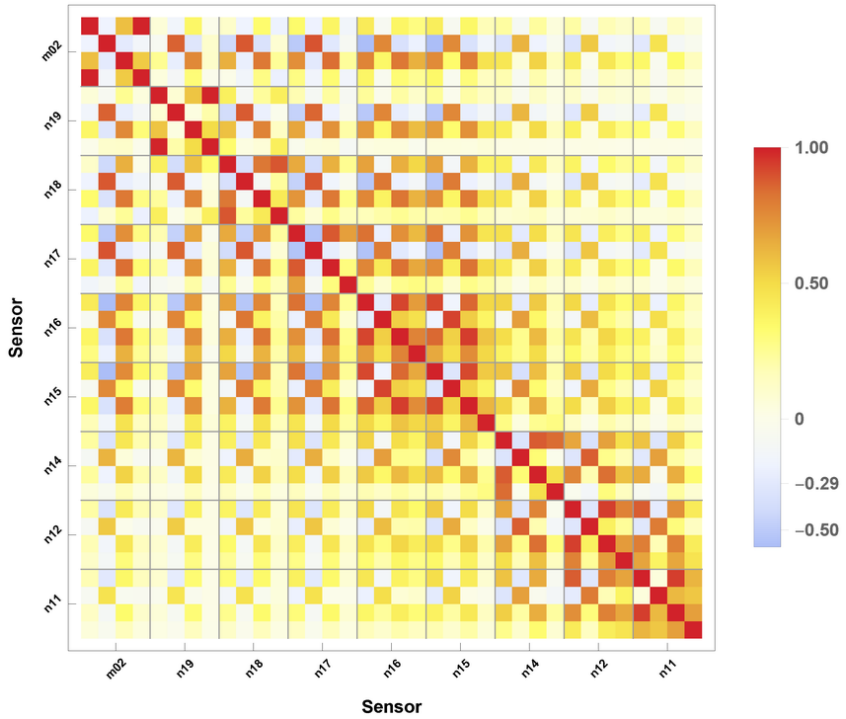
Error Correlation

What is Error Correlation?

Errors in a dataset are **not always independent** — e.g., when errors in pixels, bands instruments, or time steps are systematically related.

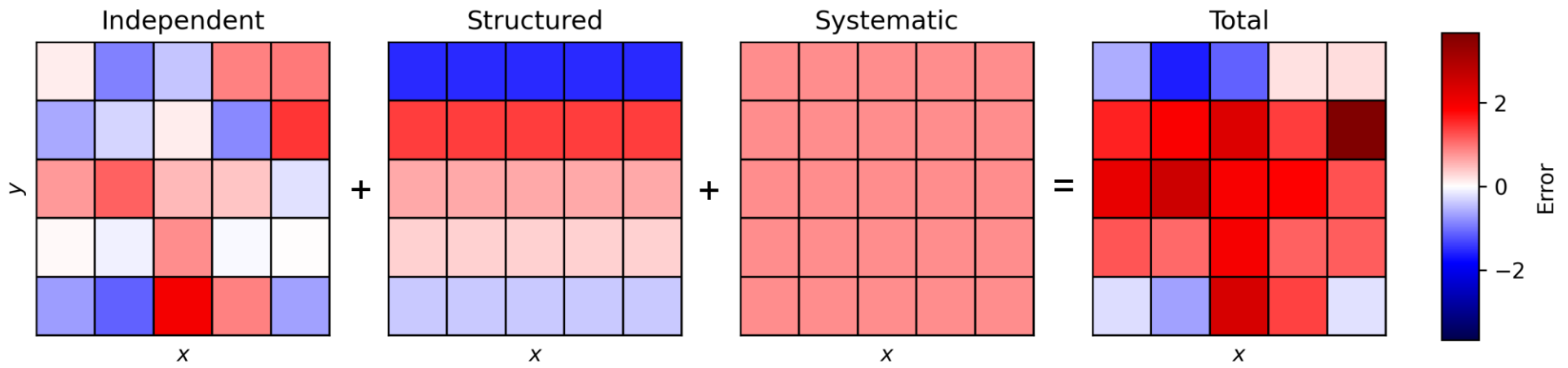
Why does it Matter?

- ❑ Bias uncertainties persist – averaging doesn't help!
- ❑ Band ratios might be off – affecting retrieval uncertainty
- ❑ Misleading confidence in trends

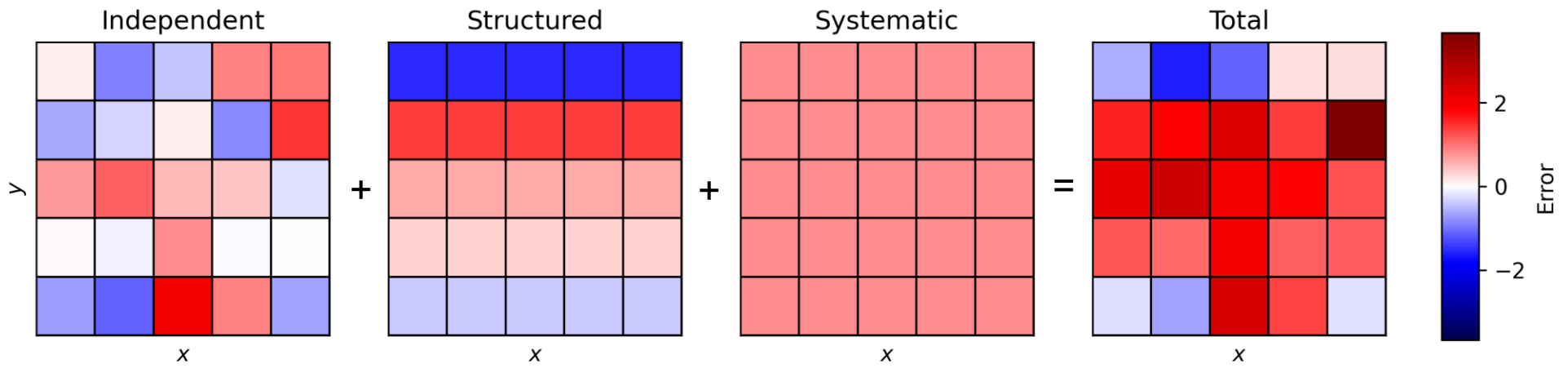


Error correlation matrix from Giering et al. 2019

ND Datasets & Error-Correlation



ND Datasets & Error-Correlation

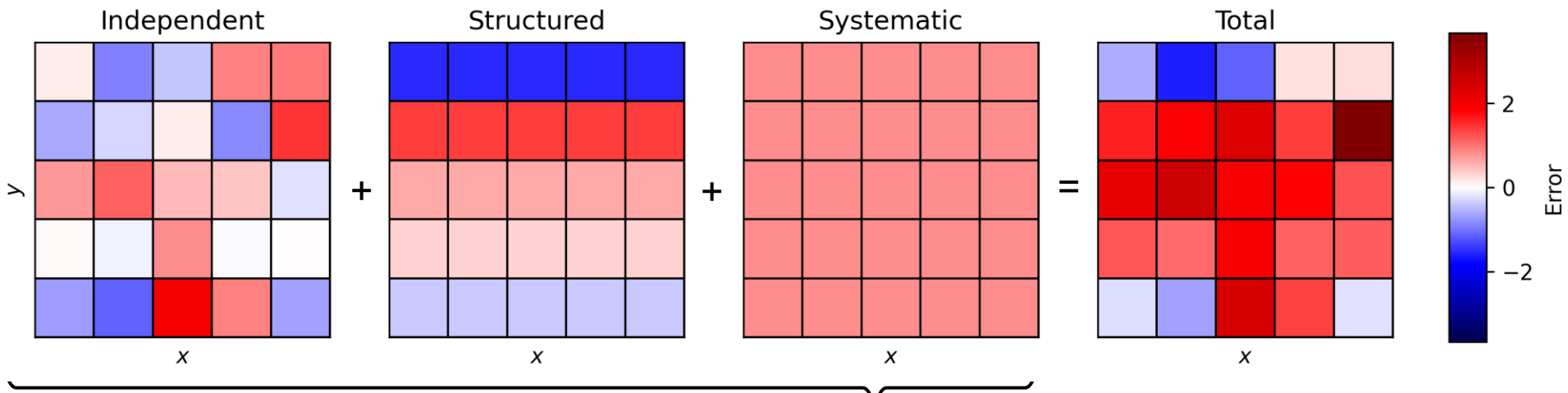


e.g., noise from detector

e.g., periodically updated correction

e.g., error on pre-flight calibration

ND Datasets & Error-Correlation



Each of these effects has the same uncertainty (u=1) – but a very different behaviour in the overall dataset! This matters!

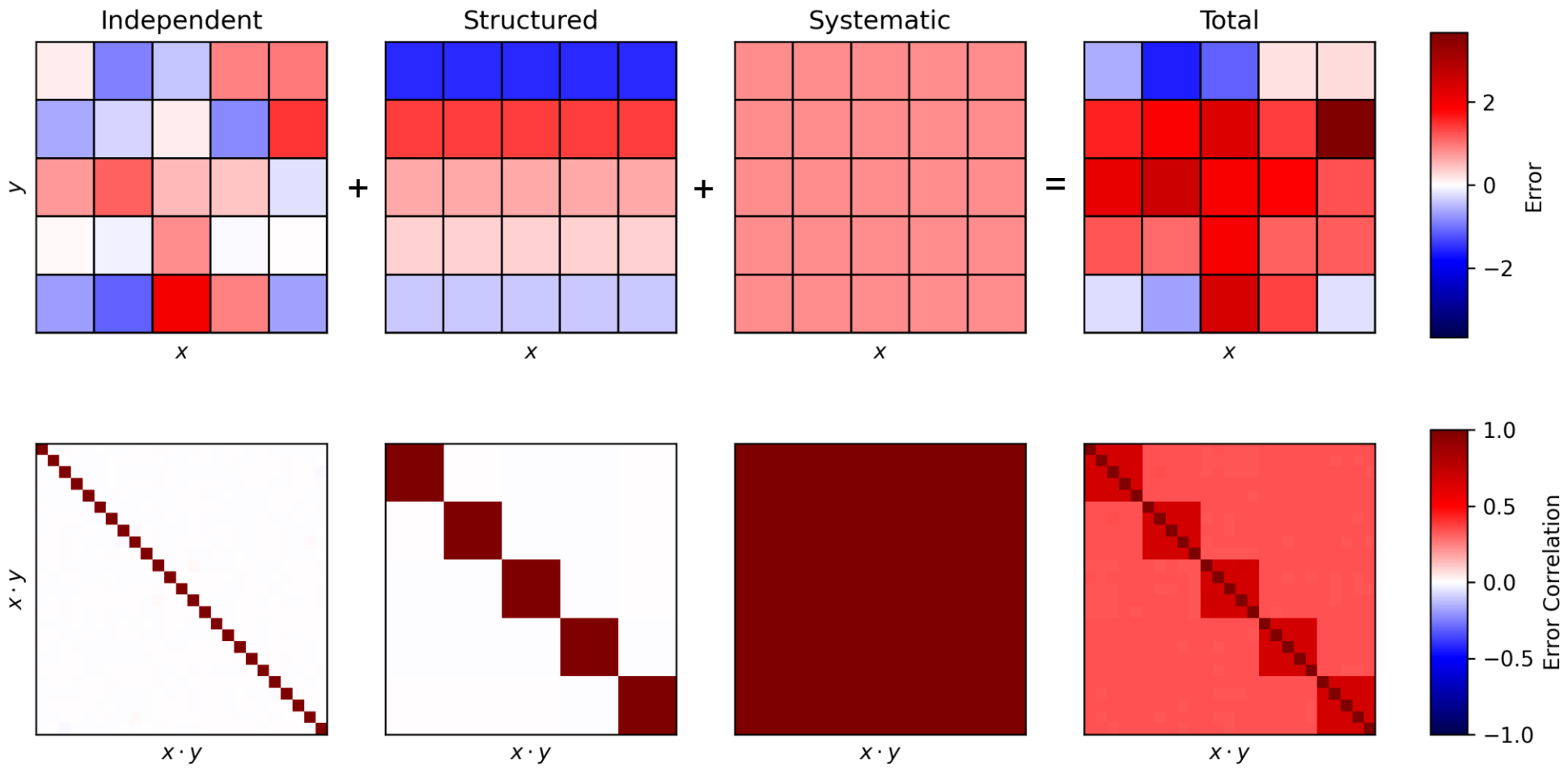
ND Datasets & Error-Correlation

Define this with an error-correlation matrix for the image, defining the cross-pixel error-correlation, $r_{i,j}$, for all pixels – label as:

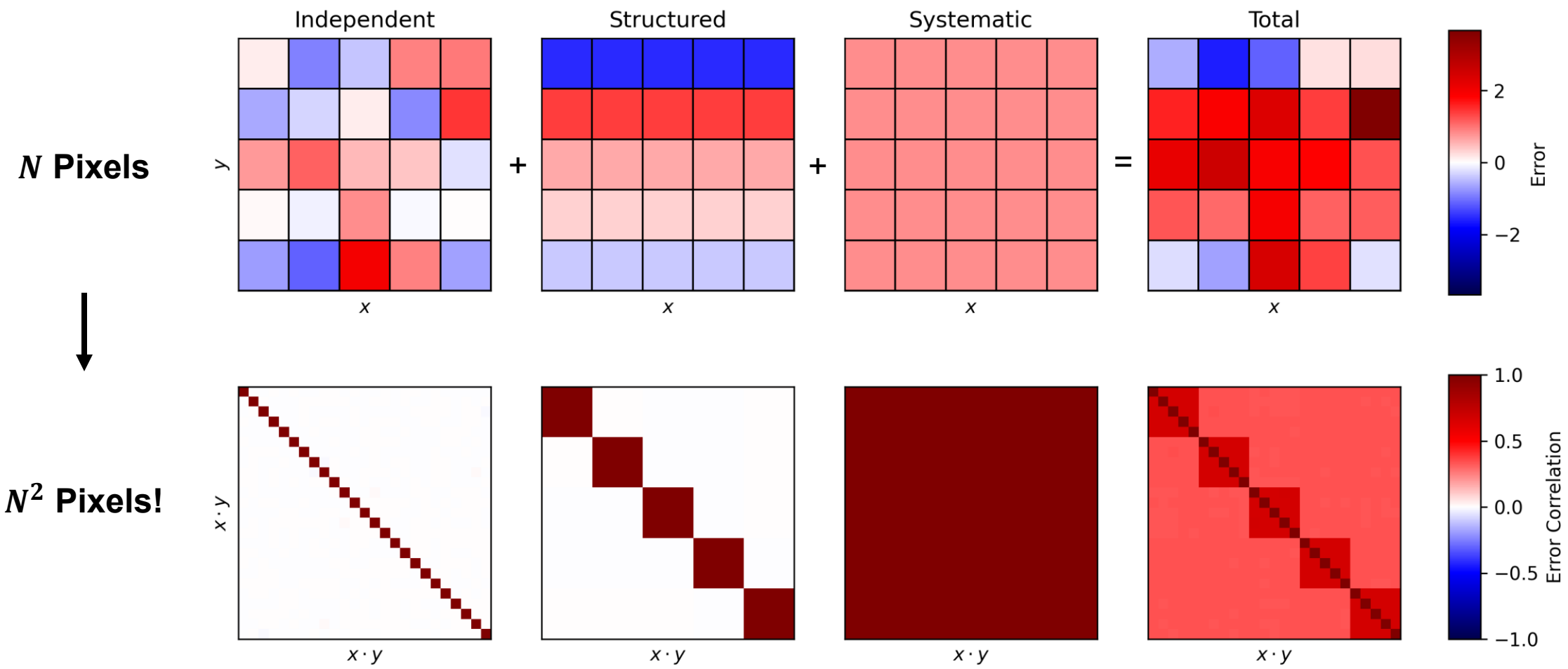
1	2	3	4	5
6	7	8	9	10
11	12	13	14	15
16	17	18	19	20
21	22	23	24	25

$$\begin{bmatrix} r_{1,1} & r_{2,1} & r_{3,1} & r_{4,1} & r_{5,1} & r_{6,1} & \cdots \\ r_{1,2} & r_{2,2} & r_{3,2} & & & & \\ r_{1,3} & r_{2,3} & r_{3,3} & & & & \\ r_{1,4} & & & \ddots & & & \\ r_{1,5} & & & & & & \\ r_{1,6} & & & & & & \\ r_{1,7} & & & & & & \\ r_{1,8} & & & & & & \\ \vdots & & & & & & \end{bmatrix}$$

ND Datasets & Error-Correlation

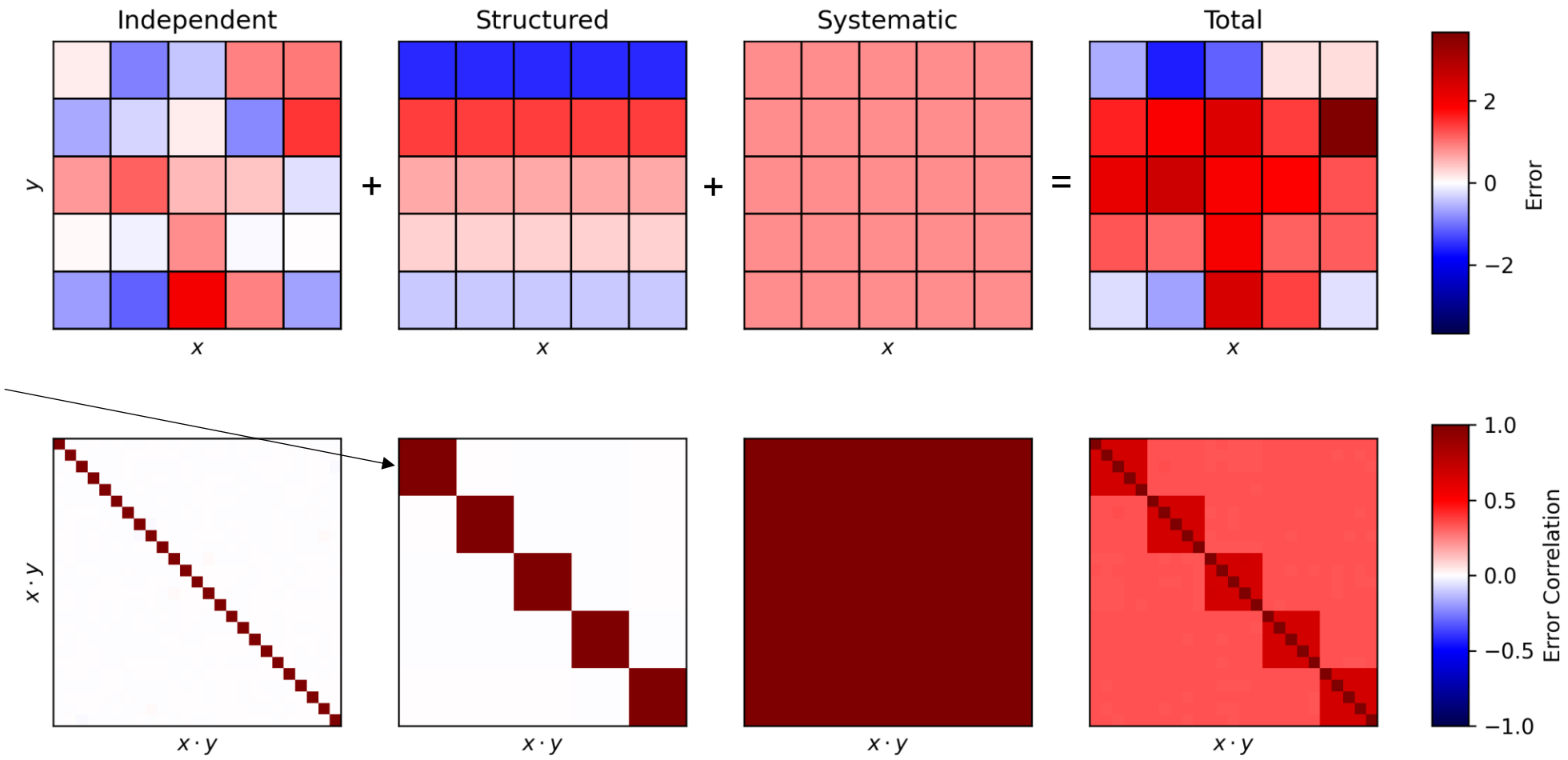


ND Datasets & Error-Correlation

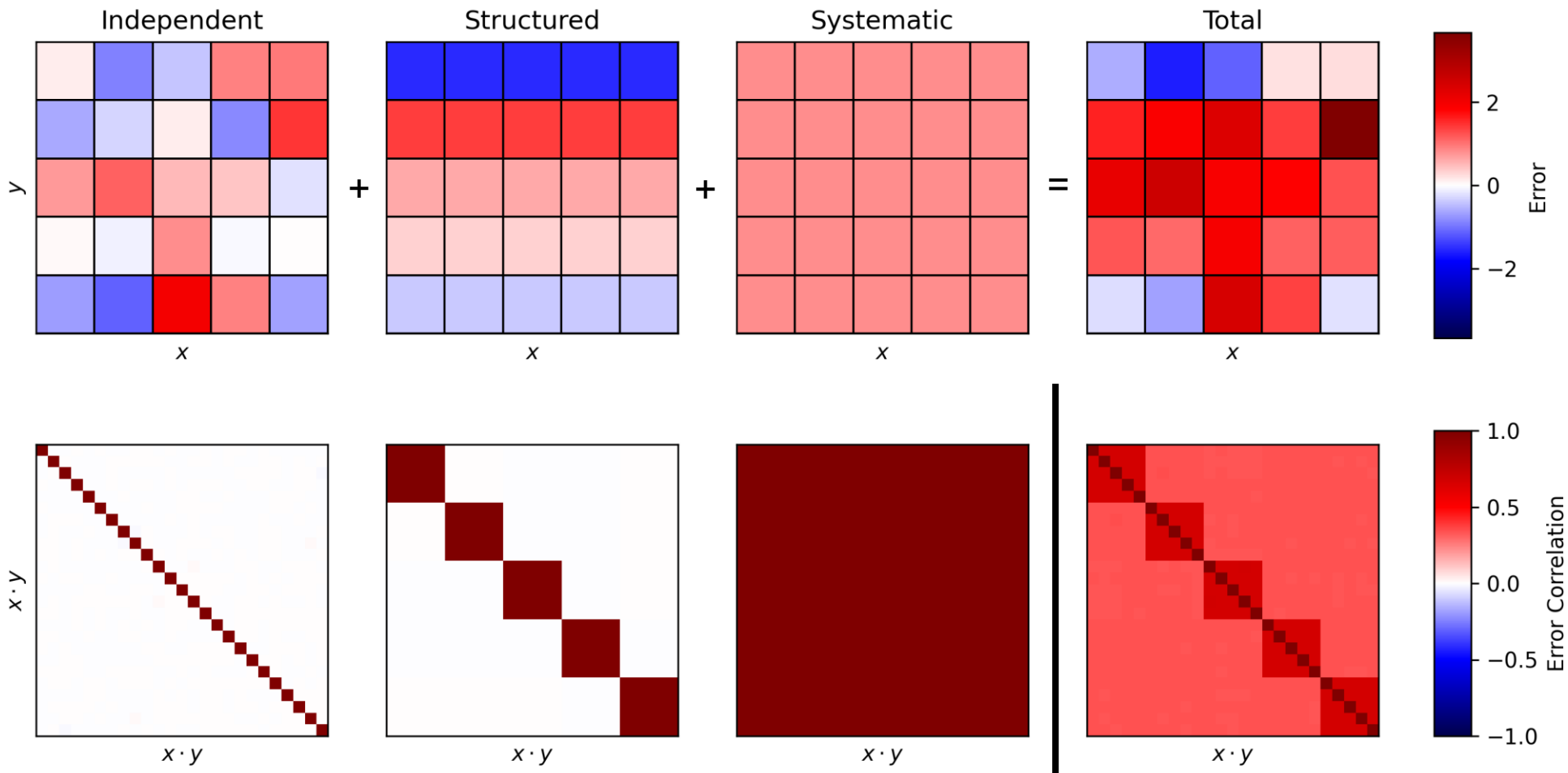


ND Datasets & Error-Correlation

Sub-matrices for systematic error-correlation within row



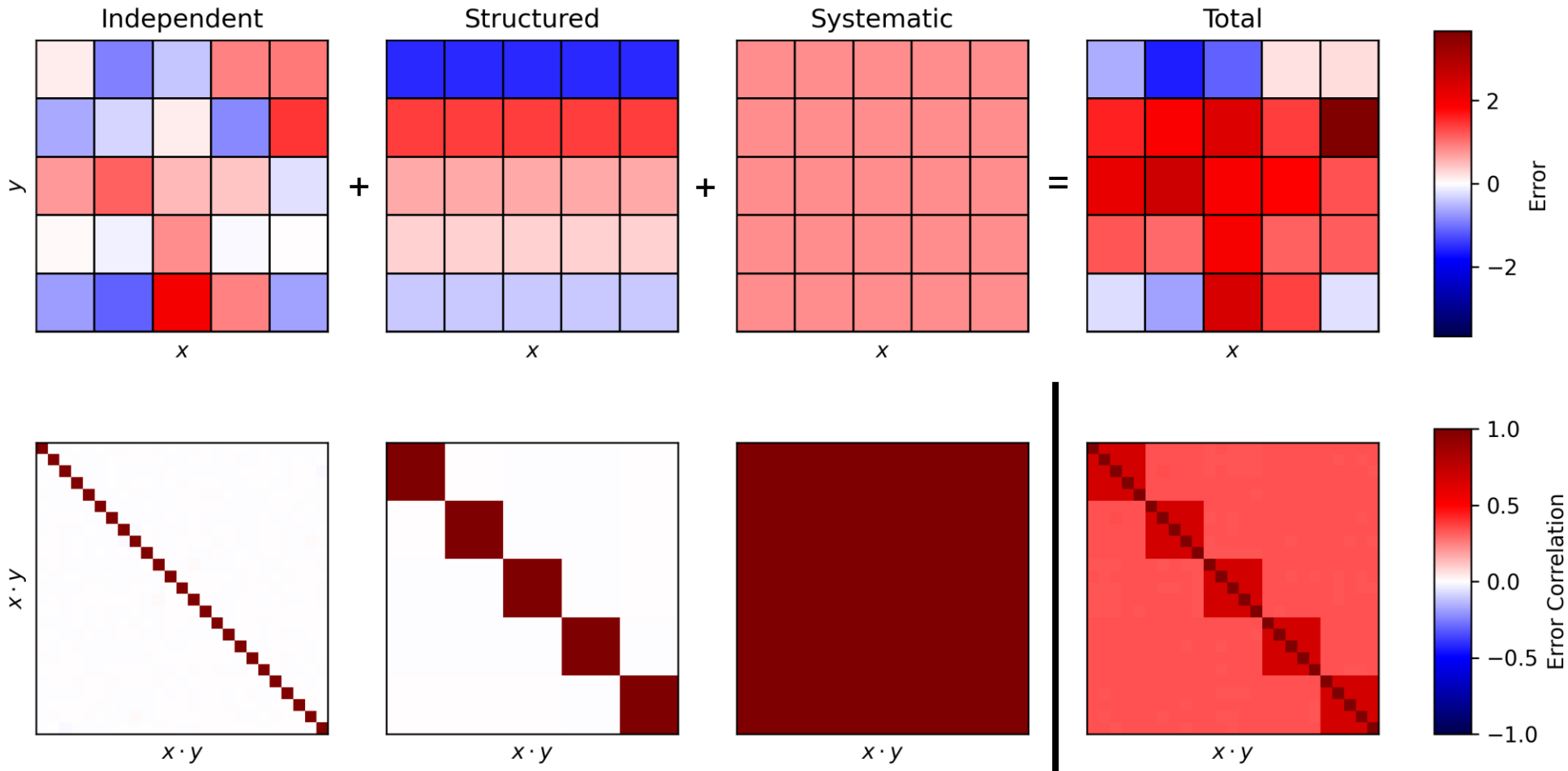
ND Datasets & Error-Correlation



- Simply parameterisable

- Parameterisable via other terms

ND Datasets & Error-Correlation



- Simply parameterisable
- One term might dominate at different scales

- Parameterisable via other terms
- Same complexity at all scales

🔍 Error Correlation

🔎 What is Error Covariance?

Combines error correlation and uncertainty

$$\boldsymbol{S = U\,R\,U^T}$$

🤷 Random, systematic and structured uncertainty

- ❑ It is the errors that are correlated, not the uncertainty values
- ❑ Random means completely uncorrelated, i.e. error correlation is identity matrix
- ❑ Systematic means fully correlated, i.e. error correlation filled with 1's

A Metrological Approach

Uncertainties are evaluated and expressed following ***QA4EO*** *Five Steps*, a framework which employs the principles of metrology.

Define the measurand and measurement function

Establish the traceability with a diagram

Evaluate each source of uncertainty and fill in an effects table

Calculate the data product and uncertainties

Record information for users

QA4EO

IDEAS-QA4EO

Fiduceo

MEASURAND
1

$$y = f(x_1, x_2, x_3) + 0$$

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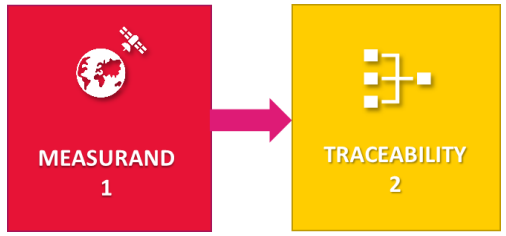
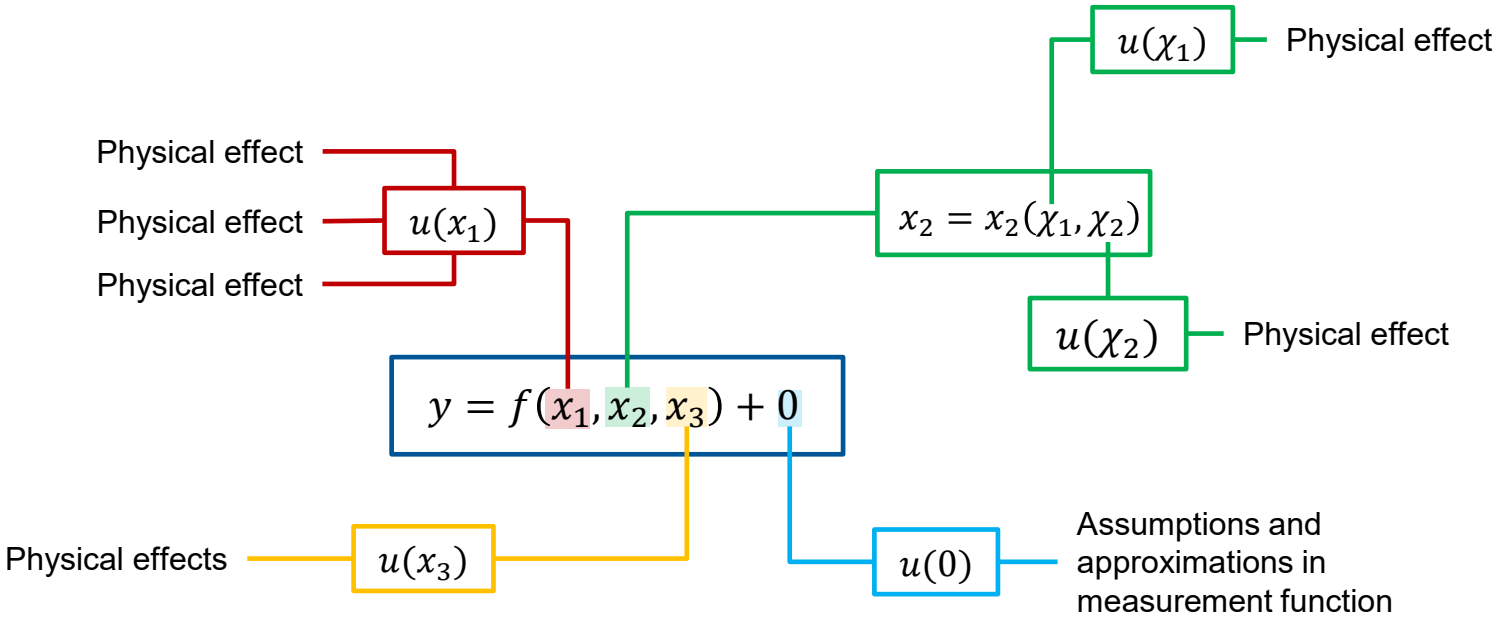
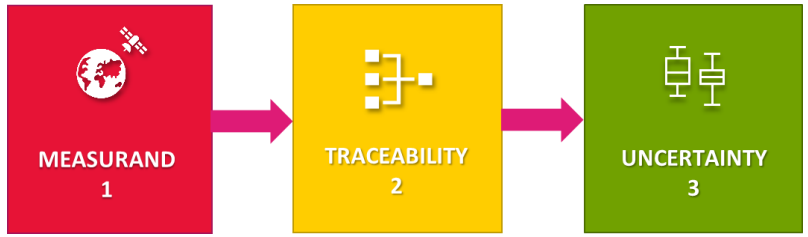
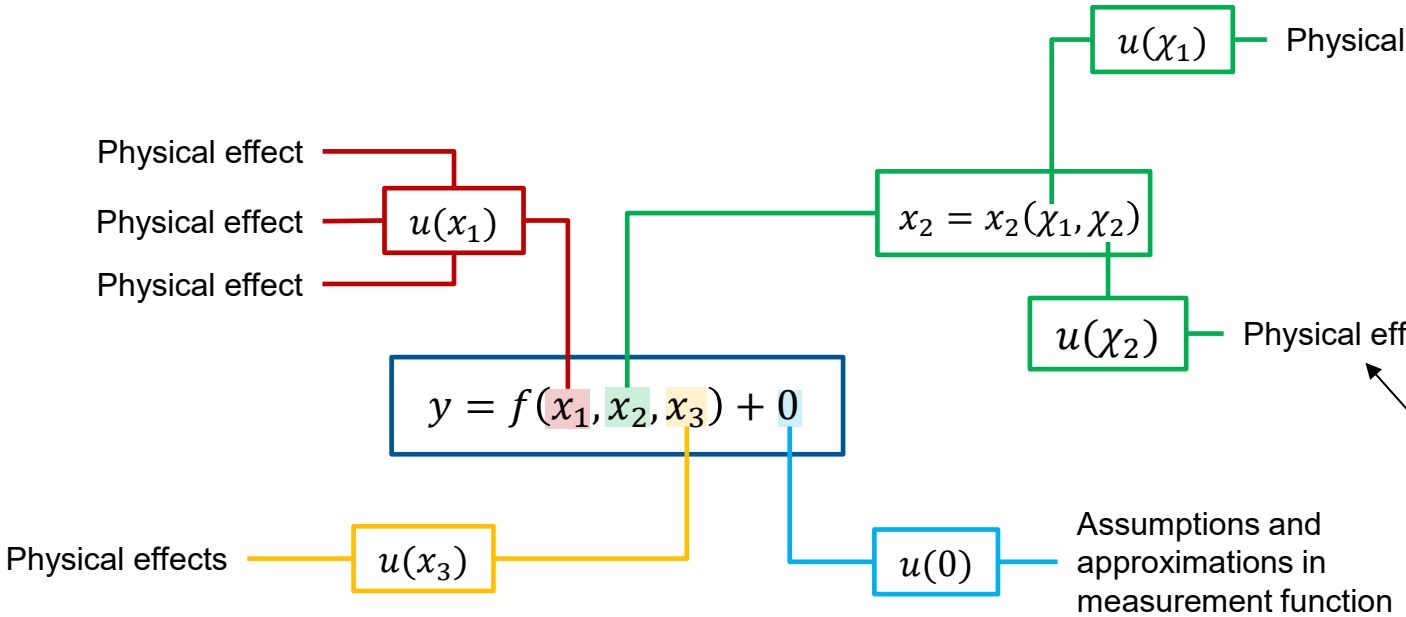
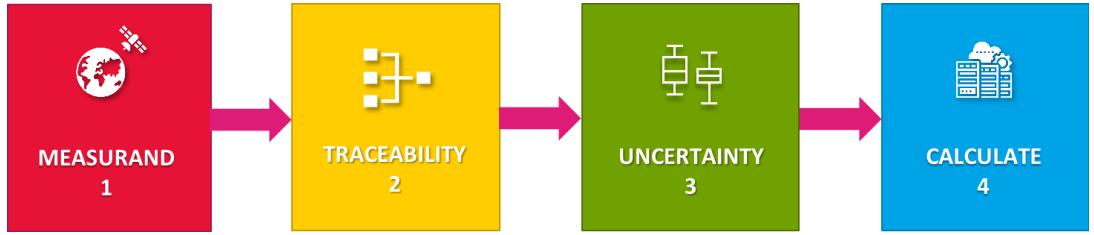

MEASURAND
1
TRACEABILITY
2


$u(\chi_1)$
Physical effect
Physical effect
Physical effect
Physical effect
$u(x_1)$
$x_2 = x_2(\chi_1, \chi_2)$
$u(\chi_2)$
Physical effect
$y = f(x_1, x_2, x_3) + 0$
Physical effects
$u(x_3)$
$u(0)$
Assumptions and approximations in measurement function

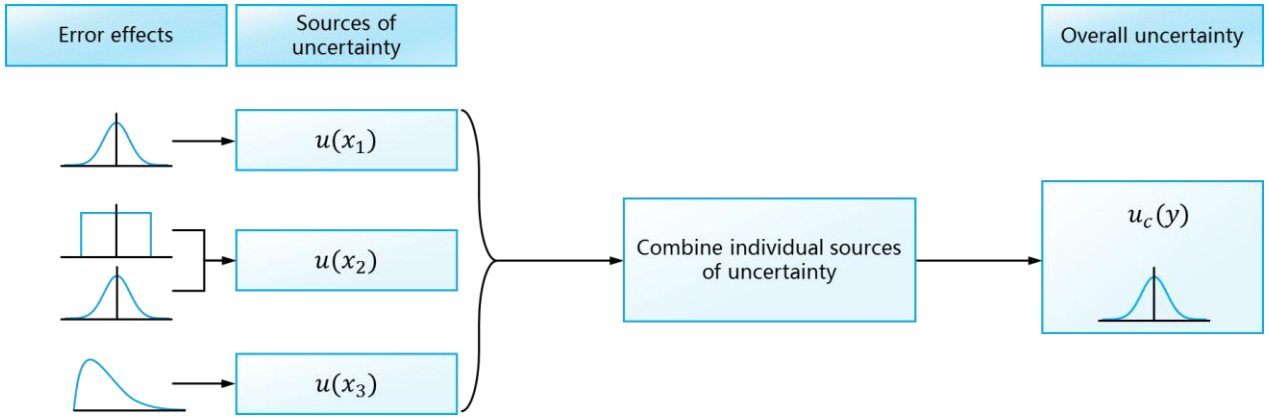




		Comments
Name of effect		A unique name
Affected term in measurement function		Name and standard symbol
Instruments in the series affected		List names
Correlation type and form	Pixel-to-pixel [pixels]	From a set of defined correlation forms
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Correlation scale	Pixel-to-pixel [pixels]	As needed to define type
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Channels/bands	List of channels / bands affected	Channel names
	Error correlation coefficient matrix	A matrix
Uncertainty	PDF shape	Functional form
	units	Units
	magnitude	
Sensitivity coefficient		Value, equation or parameterisation of sensitivity of measurand to term



punpy



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obsarray

		Comments
Name of effect		A unique name
Affected term in measurement function		Name and standard symbol
Instruments in the series affected		List names
Correlation type and form	Pixel-to-pixel [pixels]	From a set of defined correlation forms
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Correlation scale	Pixel-to-pixel [pixels]	As needed to define type
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Channels/bands	List of channels / bands affected	Channel names
	Error correlation coefficient matrix	A matrix
Uncertainty	PDF shape	Functional form
	units	Units
	magnitude	
Sensitivity coefficient		Value, equation or parameterisation of sensitivity of measurand to term

```
double u_str_temperature(x=2, y=2, time=3);
  :_FillValue = 9.969209968386869E36; // double
  :err_corr_1_dim = "x";
  :err_corr_1_form = "custom";
  :err_corr_1_units = ; // double
  :err_corr_1_params = "err_corr_str_temperature_x";
  :err_corr_2_dim = "y";
  :err_corr_2_form = "systematic";
  :err_corr_2_units = ; // double
  :err_corr_2_params = ; // double
  :err_corr_3_dim = "time";
  :err_corr_3_form = "systematic";
  :err_corr_3_units = ; // double
  :err_corr_3_params = ; // double
  :pdf_shape = "gaussian";
```

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CoMet Packages:

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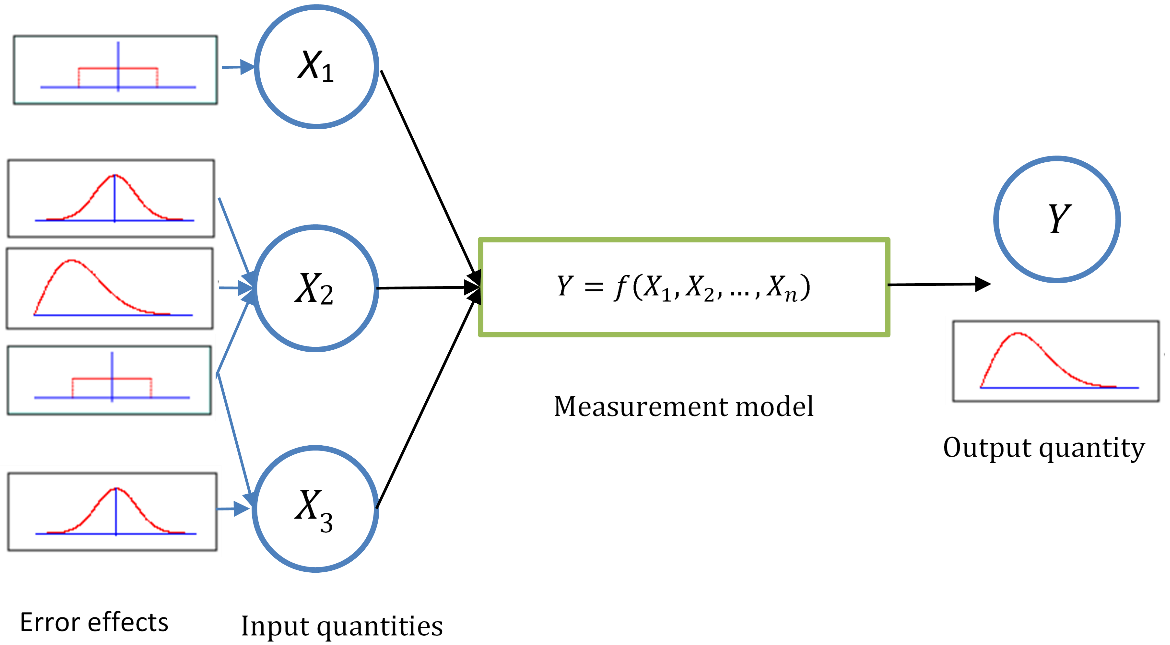
Propagating Uncertainties with punpy

- Python module for propagating **random**, **systematic** and **structured uncertainties** through any Python measurement function
- Flexible in terms of the **specified correlations** along given dimensions or between input quantities
- ***Monte Carlo*** and ***Law of Propagation of uncertainties*** methods available



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Punpy as a Standalone Tool

- Simple user **interface**:
  1. Import punpy
  2. Define measurement function
  3. Create MC or LPU object
  4. Propagate uncertainties

```
import punpy
prop=punpy.MCPropagation(10000)
unc_measurand=prop.propagate_random(measurement_func,
      [input_qt1,input_qt2],[unc_qt1,unc_qt2])
```

- **Measurement function** are defined as python functions that take arrays as input quantities and return an array as measurand

- Many optional **keywords** for flexible functionality

  - *return_corr*
  - *Corr_between*
  - *Repeat_dims*
  - *Parallel_cores*
  - *Output_vars*
  - *…*

Punpy with digital effects tables

- **punpy** interfaces with **obsarray** to make uncertainty propagation as efficient and easy to use as possible
- ***propagate_ds()*** function returns an **obsarray** dataset with combined random, systematic and structured uncertainties on measurand

```python
from punpy import MeasurementFunction

# Define your measurement function inside a subclass of MeasurementFunction
class IdealGasLaw(MeasurementFunction):
    def meas_function(self, pres, temp, n):
        return (n *temp * 8.134)/pres

# create object of the measurement function class and specify the variable names
gl = IdealGasLaw(["pressure", "temperature", "n_moles"], "volume", yunit="m^3")

# propagate uncertainties on the input quantities in ds to measurand in ds_y
ds_y = gl.propagate_ds(ds)
```

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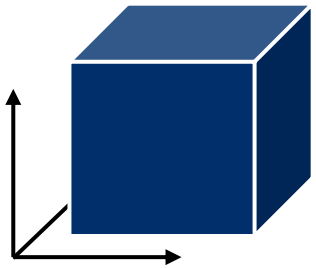
CoMet Packages:

UNC Specification

obsarray

Uncertainty Variable Metadata

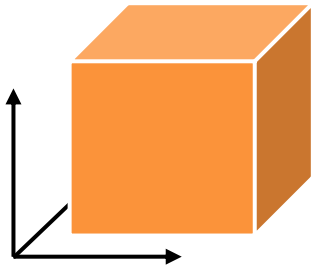
Observation Variables

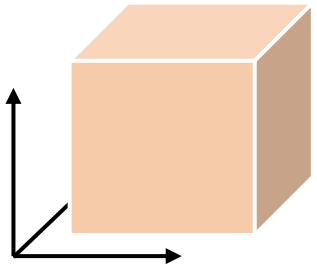


Metadata:
- Uncertainty Components

associated with

Uncertainty Variables





...

Metadata:
- **PDF Shape** (gaussian, …)
- **Units** (abs. or rel.)
- **Error-Correlation**…

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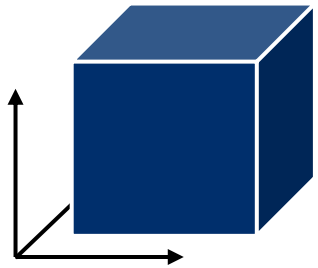
UNC Specification

obsarray

🌡️ Example – Temperature Dataset

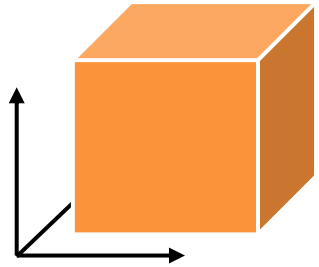
Observation Variables



temperature

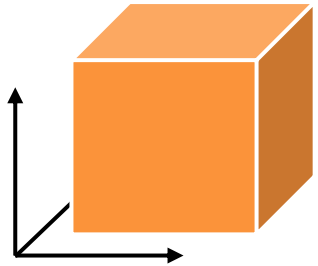
associated with

Uncertainty Variables



u_noise

Metadata:
- PDF Shape – “gaussian”
- Units – %
- Error-Correlation:
  - All dims - Random



u_calibration

Metadata:
- PDF Shape – “rectangular”
- Units – “K”
- Error-Correlation:
  - **x, y** – systematic
  - **time** – defined by matrix

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UNC Specification

obsarray

🌡️ Example – Temperature Dataset

```
variables:
  float temperature(time, lat, lon);
    temperature:unc_comps=["u_calibration", "u_noise"];
    temperature:units="K"
  float u_calibration(time, lat, lon);
    u_calibration:units="K";
    u_calibration:pdf_shape="rectangular";
    u_calibration:err_corr_dim1_name=["lat", "lon"];
    u_calibration:err_corr_dim1_form="systematic";
    u_calibration:err_corr_dim2_name="time";
    u_calibration:err_corr_dim2_form="err_corr_matrix";
    u_calibration:err_corr_dim2_params=["err_corr_calibration_time"];
  float u_noise(time, lat, lon);
    u_calibration:err_corr_dim1_name=["time", "lat", "lon"];
    u_calibration:err_corr_dim1_form="random";
  float err_corr_calibration_time(time, time);
```

Measurement data handling in Python

- **obsarray** is an extension to **xarray** to support defining, storing and interfacing with measurement data – using the UNC specification.
- Also has functionality for defining flags following **CF Conventions**.
- It is designed to work well with **netCDF** files and for the **Earth Observation** community.

Plugs straight into punpy for propagation through measurement functions!

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CoMet Application Examples

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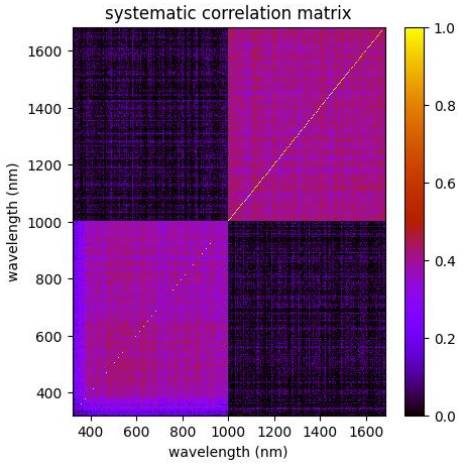
CoMet Toolkit in Action

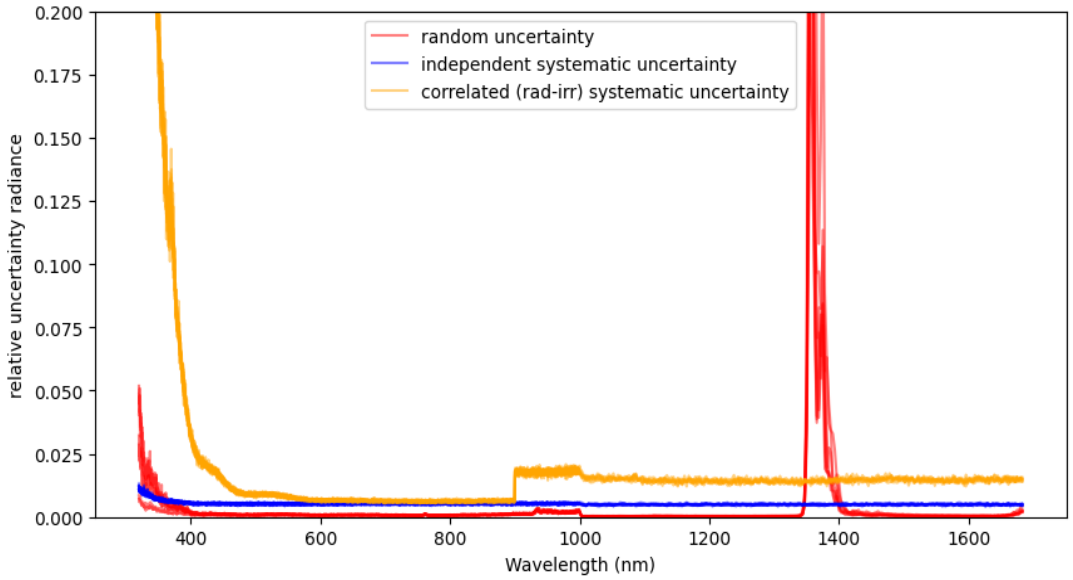
- Validated against **NIST** uncertainty engine:
  https://colab.research.google.com/github/comet-toolkit/comet_training/blob/main/NIST_example.ipynb

- *CoMet* is used in various other projects, such as **QA4EO**, **HYPERNETS**, **CHIME L2**, **FLEX** validation, **TRUTHS** science studies, **LIME**, **FRM4SOC**, **RPV4PICS**

- **Example** from *hypernets_processor*:

  Hypernets is an automated network of in-situ instruments measuring reflectance for L2 satellite validation





CoMet Release

- ❑ V1.0 of Comet toolkit has been released as **open source** toolkit:
  - www.comet-toolkit.org
  - github.com/comet-toolkit

- ❑ Accompanied by training material (**Jupyter** notebooks hosted on google colab):
  - www.comet-toolkit.org/examples

- ❑ Documentation & ATBD for individual tools:
  - obsarray.readthedocs.io/en/latest/
  - punpy.readthedocs.io/en/latest/
  - comet-maths.readthedocs.io/en/latest/

📈 Outlook

- **Current release** will be presented De Vis & Hunt (in prep)

- Looking to continue to expand the use cases the developed tools
  - Aiming to enable uncertainty propagation through **any python measurement function**
  - 📧 Please get in touch if you are interested!

- This has been our first step into this way of working, **many more ideas in a roadmap** to building up a comprehensive set of tools
  - e.g. retrieval tool/optimisation, BRDF tool, Look-up tables for faster processing, etc.

✅ Summary

- The **CoMet toolkit** is an open-source software project to develop Python tools for the handling of error-covariance information in the analysis of measurement data
- This toolkit is based on **robust metrology**, and makes dealing with complexities of uncertainties much easier
- Includes **obsarray**, **punpy** & **comet_maths** as initial offering, to be extended
- These tools are already being used operationally in various projects (e.g. Hypernets)

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Exercises

- Please go to www.comet-toolkit.org/user-guide/training/

Mentimeter

Code: 1687 1279

Today's Exercises

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