Ensemble Sensitivity Analysis

A Practical Introduction

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StuMeTa 2021

Overview

- 3 Hours
- 3 Parts:
    1. Introduction (theory) and sensitivity pattern quiz
    2. Practical considerations and normalization (hands-on)
    3. Example from the literature (hands-on)

You can **interrupt me at any time**, please ask questions!

Part I

- Sensitivity Analysis
- From Ensemble Regression to ESA
- Sensitivity Maps: Construction, Interpretation
- Quiz

Sensitivity Analysis

(How (much)) does T change when S changes?

Sensitivity Analysis

(How (much)) does T change when S changes?

Examples:

- How do initial condition errors affect forecast performance?
- Where should I add observations to improve a forecast?
- Where and when did an error in the forecast first develop?
- Which region should I pay attention to in the next forecast?
- How are different state variables related?

Sensitivity Analysis: Techniques

- **Climatological analysis** (e.g. composites)

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- **Deterministic modelling**
  - Data denial
  - Relaxation
  - Adjoint sensitivities

Sensitivity Analysis: Techniques

- **Climatological analysis** (e.g. composites)
- **Deterministic modelling**
  - Data denial
  - Relaxation
  - Adjoint sensitivities
- **Probabilistic modelling**
  - Ensemble Sensitivity Analysis
  - Clustering

Ensemble Synoptic Analysis

- Introduced as general term (Hakim and Torn 2008)
- **Regression techniques**
- Extract information from ensemble forecasts

Idea:

- Apply regression “**along**” the ensemble/**member dimension**
- In ML terms: the **ensemble** provides the **training dataset**

Ensemble Regression

Multivariate Regression

- Each ensemble member provides one data point for “training”

Steps:

1. Pick a **target** / forecast metric(s) / predictand(s): $\boldsymbol{T}$
2. Pick a **source** / analysis field(s) / predictors: $\boldsymbol{S}$
3. Train a **regression model** with ensemble: $\boldsymbol{T} = \mathrm{f}\left(\boldsymbol{S}\right)$
4. Analyse model or use it for perturbation experiments

Ensemble Regression: Linear Model

Perturbations: $\hat{\boldsymbol{S}} = \boldsymbol{S} - \bar{\boldsymbol{S}}$ and $\hat{\boldsymbol{T}} = \boldsymbol{T} - \bar{\boldsymbol{T}}$

Linear Model: $\hat{\boldsymbol{T}} = \mathrm{L}\hat{\boldsymbol{S}}$

Ensemble Regression: Linear Model

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Linear Model: $\hat{\boldsymbol{T}} = \mathrm{L}\,\hat{\boldsymbol{S}}$ (right multiply by $\hat{\boldsymbol{S}}^T$)

$\Leftrightarrow$ $\hat{\boldsymbol{T}}\,\hat{\boldsymbol{S}}^T = \mathrm{L}\,\hat{\boldsymbol{S}}\,\hat{\boldsymbol{S}}^T$

Ensemble Regression: Linear Model

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$$\Leftrightarrow \quad \hat{\boldsymbol{T}}\,\hat{\boldsymbol{S}}^T = \mathrm{L}\,\hat{\boldsymbol{S}}\,\hat{\boldsymbol{S}}^T$$

$$\Leftrightarrow \quad \operatorname{cov}\left(\boldsymbol{T}, \boldsymbol{S}\right) = \mathrm{L}\,\operatorname{cov}\left(\boldsymbol{S}, \boldsymbol{S}\right)$$

Ensemble Regression: Linear Model

Perturbations: $\hat{\boldsymbol{S}} = \boldsymbol{S} - \bar{\boldsymbol{S}}$ and $\hat{\boldsymbol{T}} = \boldsymbol{T} - \bar{\boldsymbol{T}}$

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$$\Leftrightarrow \quad \mathrm{cov}\left(\boldsymbol{T}, \boldsymbol{S}\right) = \mathrm{L}\ \mathrm{cov}\left(\boldsymbol{S}, \boldsymbol{S}\right)$$

$$\Rightarrow \quad \mathrm{L} = \mathrm{cov}\left(\boldsymbol{T}, \boldsymbol{S}\right)\ \mathrm{cov}\left(\boldsymbol{S}, \boldsymbol{S}\right)^{-1}$$

Ensemble Regression: Sensitivity

Perturbation-based workflow:

1. Select source and target variables
2. Determine L for $\hat{\boldsymbol{S}}$, $\hat{\boldsymbol{T}}$ relationship with ensemble
3. Prescribe a perturbation $\hat{\boldsymbol{S}}$
4. Examine the target response $\hat{\boldsymbol{T}} = \mathrm{L}\hat{\boldsymbol{S}}$

$$\hat{\boldsymbol{S}} = \boldsymbol{S} - \bar{\boldsymbol{S}} \longrightarrow \boxed{\mathrm{L}} \longrightarrow \hat{\boldsymbol{T}} = \boldsymbol{T} - \bar{\boldsymbol{T}}$$

Ensemble Regression: Issues

- **Ill conditioned** (large state space, small ensemble)
- Perturbation-based workflow **doesn’t scale** well
  - Trial-and-error approach difficult to automate
  - Hard to visualize effectively

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Is it possible to **visualize L directly?**

→ **ESA: yes**, but we have to simplify

Ensemble Sensitivity Analysis

Reminder: $\mathrm{L} = \operatorname{cov}(\boldsymbol{T}, \boldsymbol{S}) \operatorname{cov}(\boldsymbol{S}, \boldsymbol{S})^{-1}$

Simplifications:

1. Restriction to scalar target: $\boldsymbol{T} \rightarrow \boldsymbol{t}$

Ensemble Sensitivity Analysis

Reminder: $\mathrm{L} = \mathrm{cov}\left(\boldsymbol{T}, \boldsymbol{S}\right)\, \mathrm{cov}\left(\boldsymbol{S}, \boldsymbol{S}\right)^{-1}$

Simplifications:

1. Restriction to scalar target: $\boldsymbol{T} \rightarrow \boldsymbol{t}$
2. Ignore off-diagonal elements in $\mathrm{cov}\left(\boldsymbol{S}, \boldsymbol{S}\right)$

$$\mathrm{cov}\left(\boldsymbol{S}, \boldsymbol{S}\right)^{-1} \rightarrow \begin{pmatrix} \sigma_{\boldsymbol{s}_1}^{-2} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_{\boldsymbol{s}_m}^{-2} \end{pmatrix}$$

Ensemble Sensitivity Analysis

Simplifications:

1. Restriction to scalar target: $\boldsymbol{T} \rightarrow \boldsymbol{t}$
2. Ignore off-diagonal elements in $\operatorname{cov}(\boldsymbol{S}, \boldsymbol{S})$

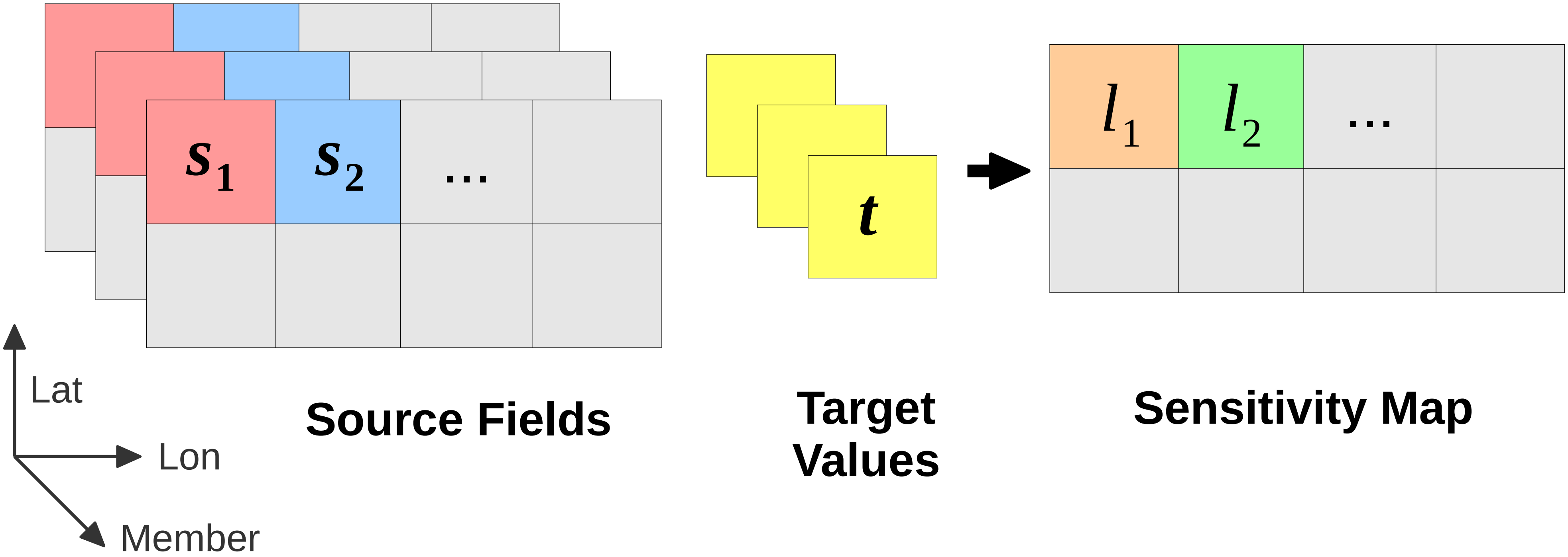
➔ **independent univariate regression** for every $\boldsymbol{s_i}$:

$$\mathrm{L} = \underbrace{\begin{pmatrix} l_1 & \cdots & l_m \end{pmatrix}}_{\text{Same size as source!}} \quad \text{where} \quad l_i = \frac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}^2} = \frac{\partial t}{\partial s_i}$$

Sensitivity Map: Construction

Plot the slope at every gridpoint!

$$l_i = \frac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s}_i)}{\sigma_{s_i}^2} = \frac{\partial t}{\partial s_i}$$



Sensitivity Map: Interpretation

Plot the slope at every gridpoint!

$$l_i = \frac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}^2} = \frac{\partial t}{\partial s_i}$$

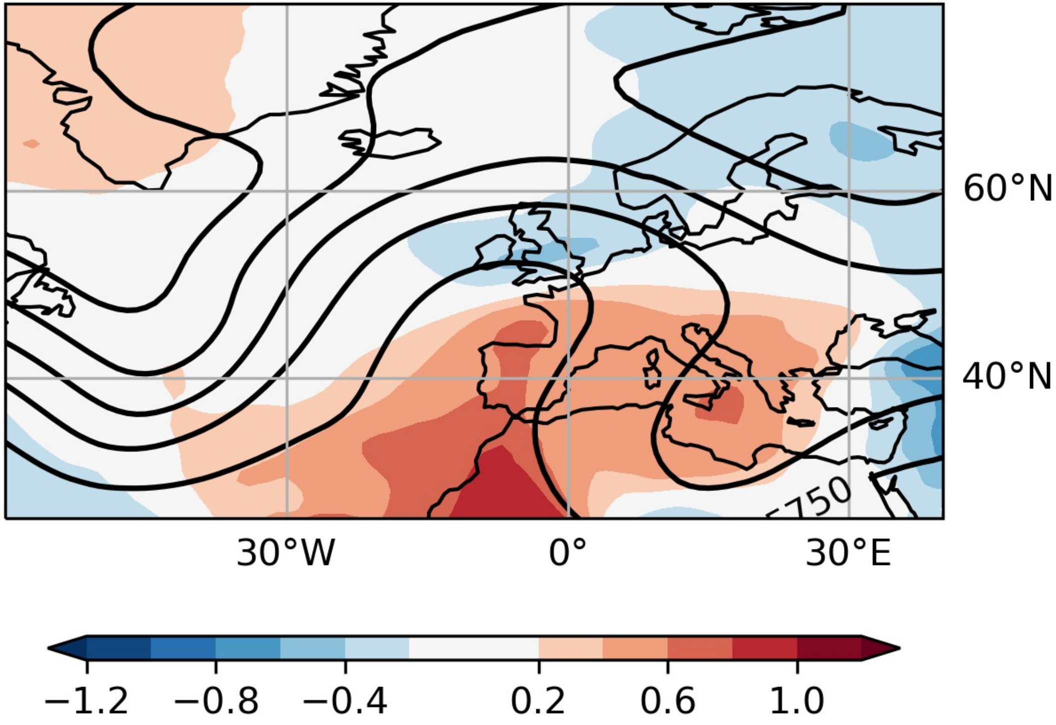
How (much) does T change when S changes?

- **Slope > 0**: larger $s_i \rightarrow$ larger t
- **Slope < 0**: larger $s_i \rightarrow$ smaller t

Visualization as map: spatial localization

- Directly read off response of t at every gridpoint

Sensitivity Map: Example



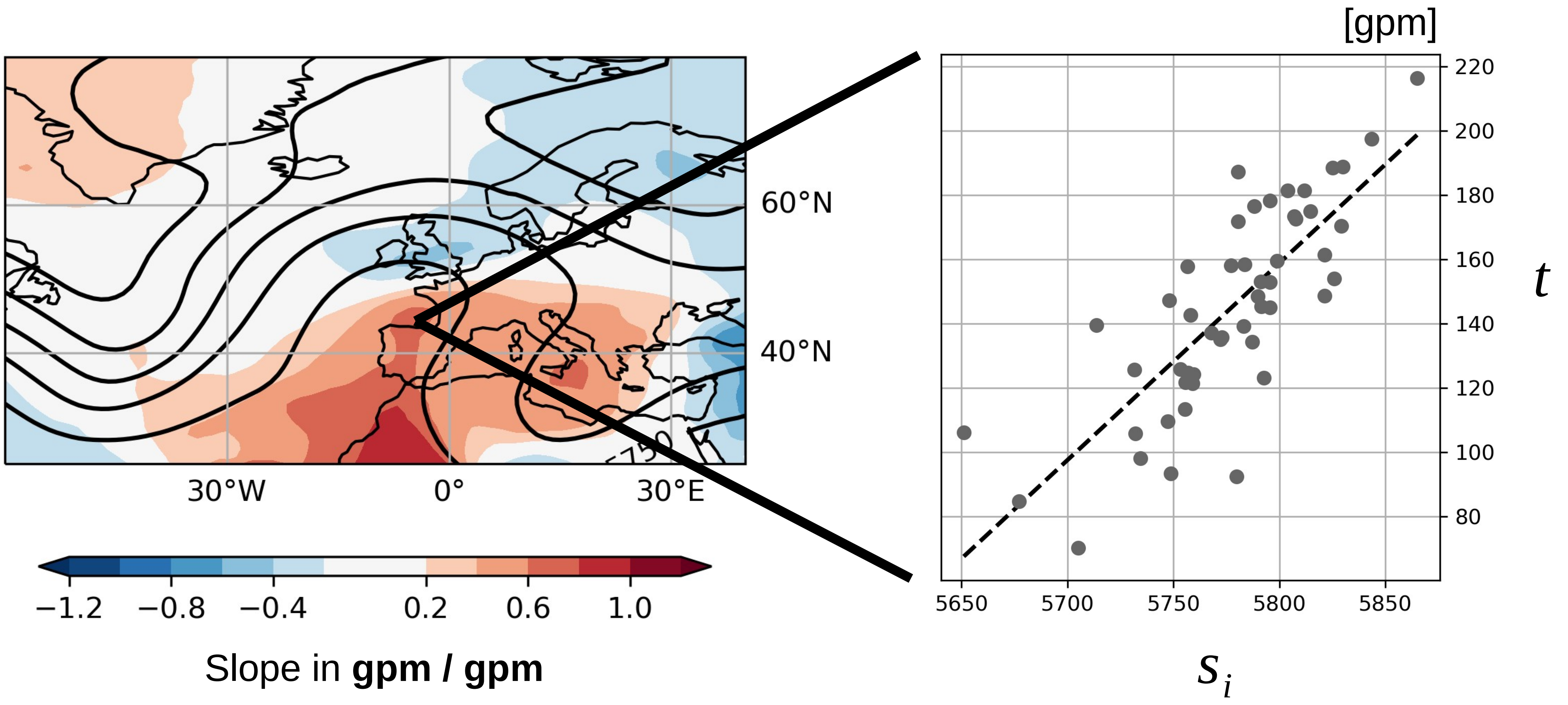
Slope in **gpm / gpm**

- **Slope > 0**
  larger $s_i \rightarrow$ larger t
- **Slope < 0**
  larger $s_i \rightarrow$ smaller t

Here:

- t = forecast error
- s_i = 500 hPa Geopot.

Sensitivity Map: Example



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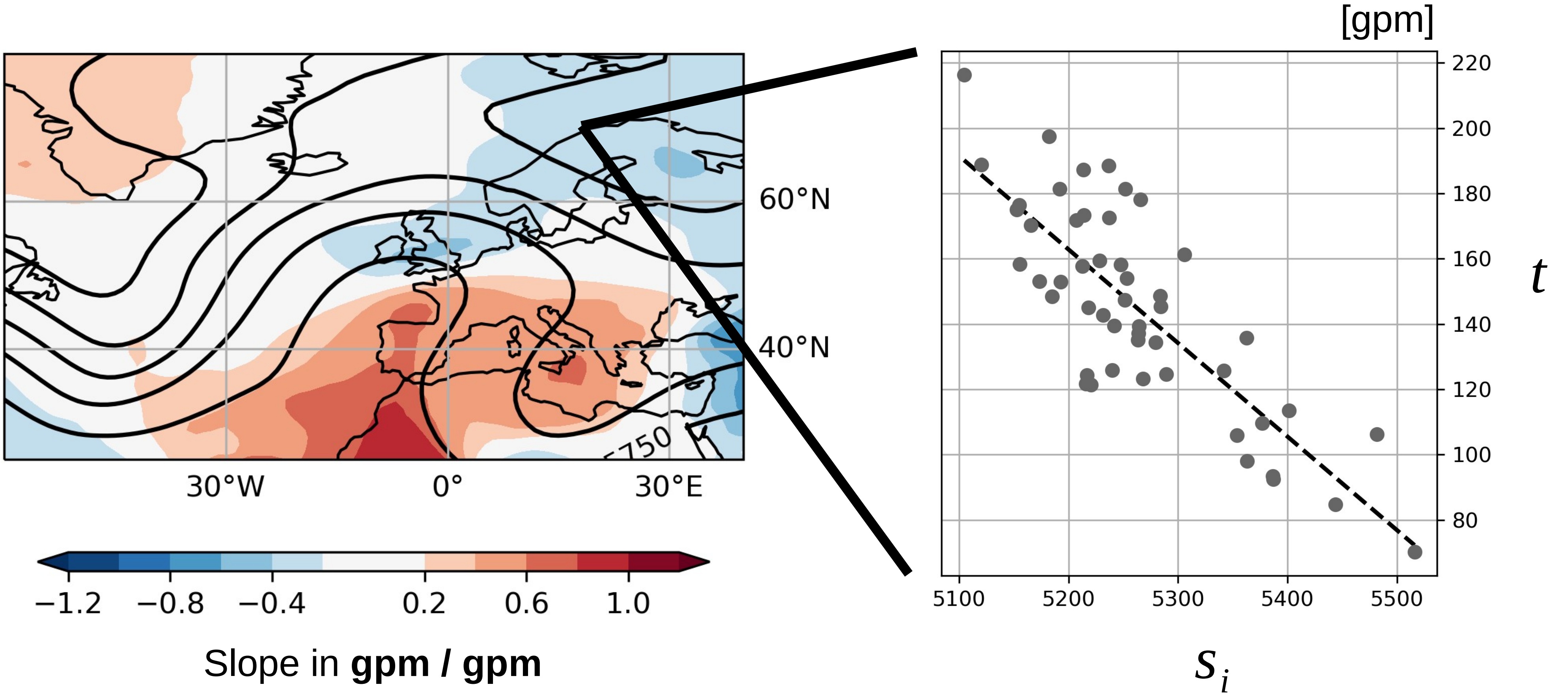
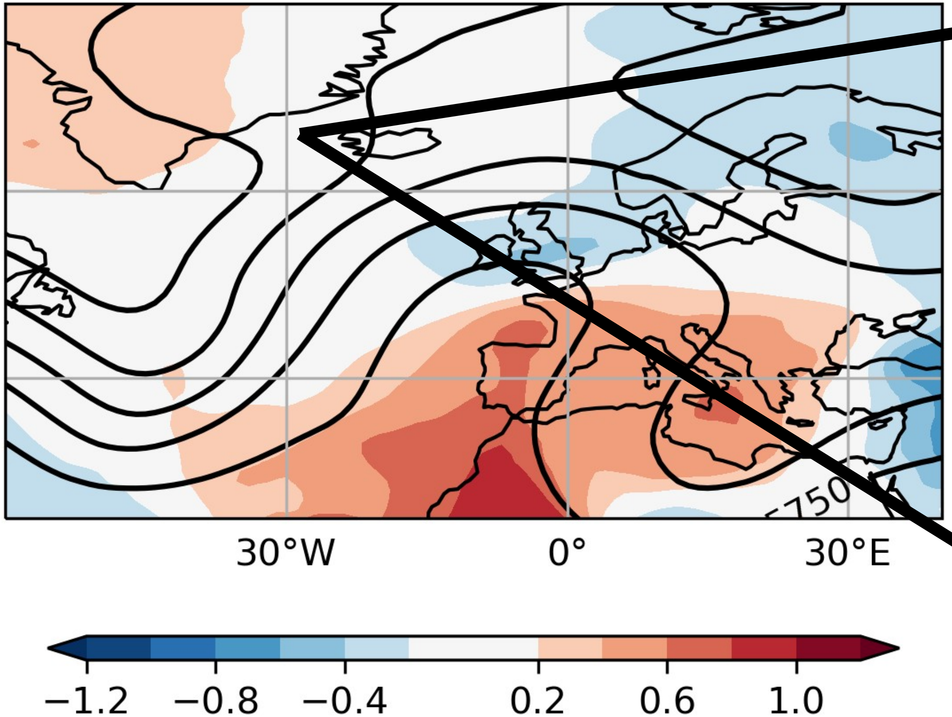
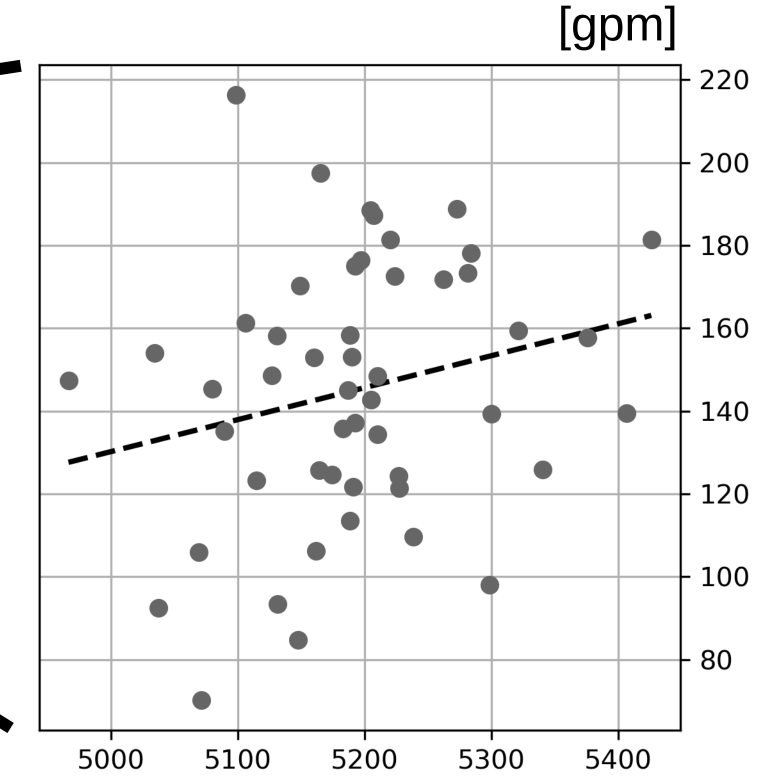


Sensitivity Map: Example



Slope in **gpm / gpm**



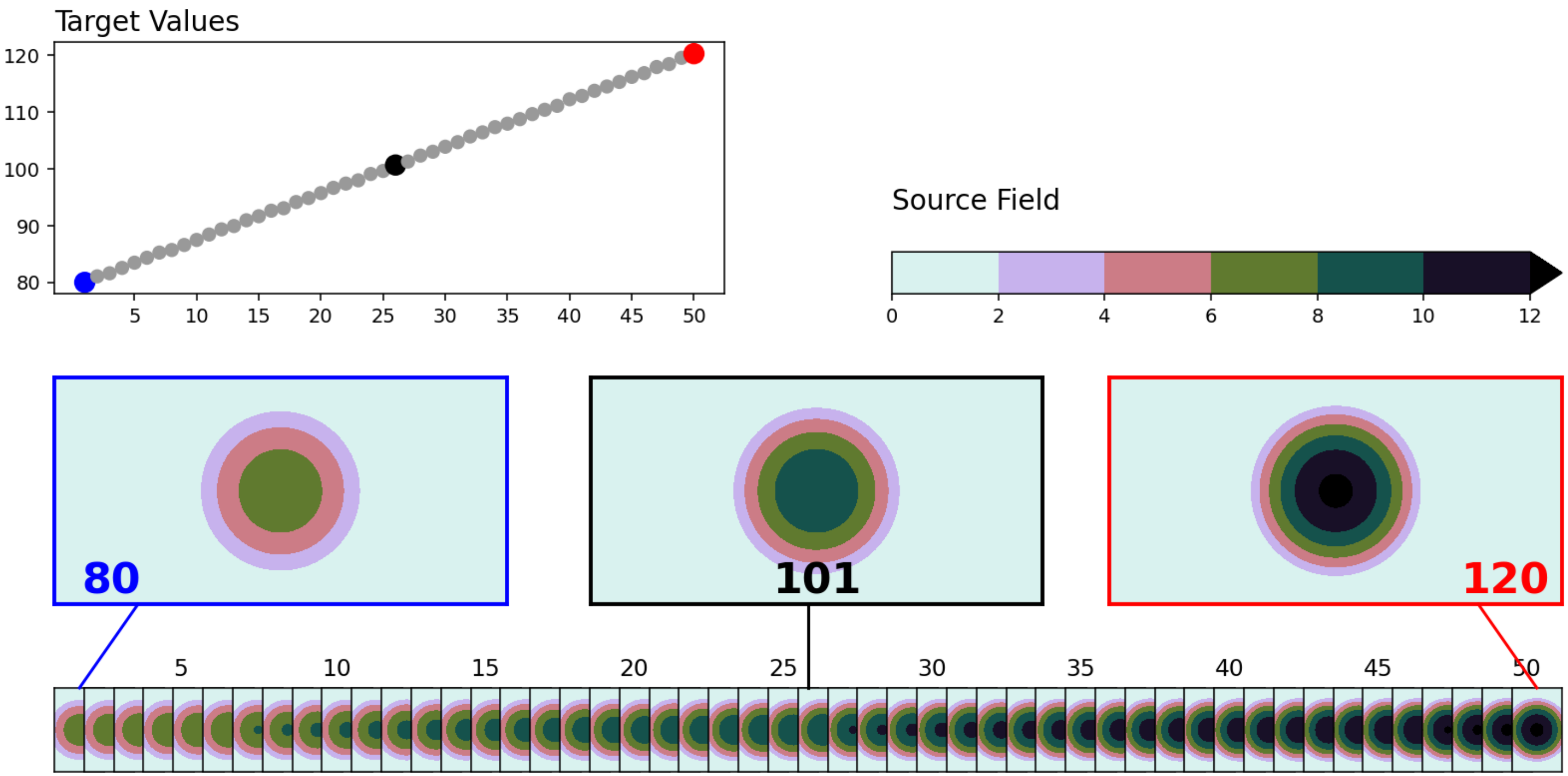
t

s_i

Hands-on

Sensitivity Pattern Quiz

A: Blob Amplitude Uncertainty



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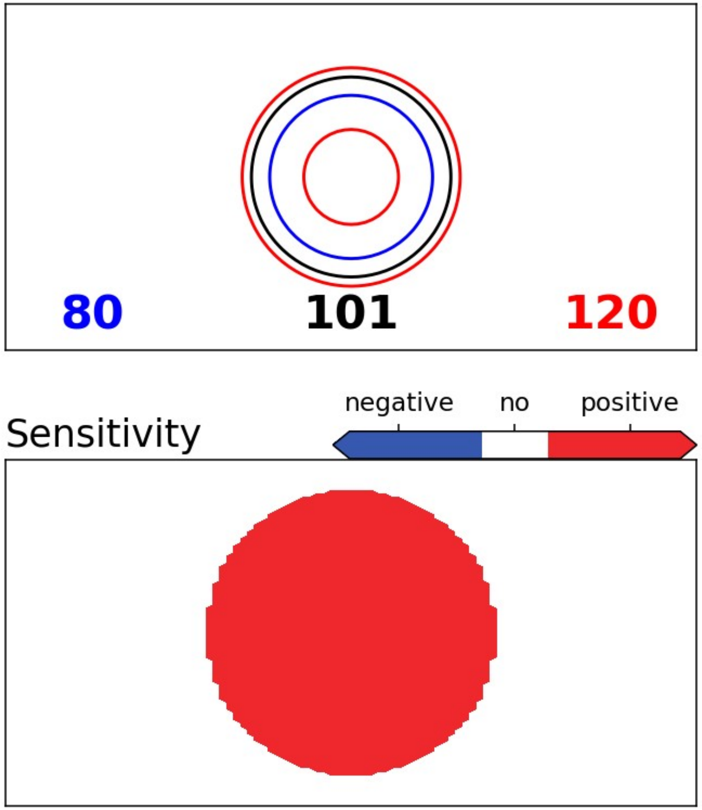

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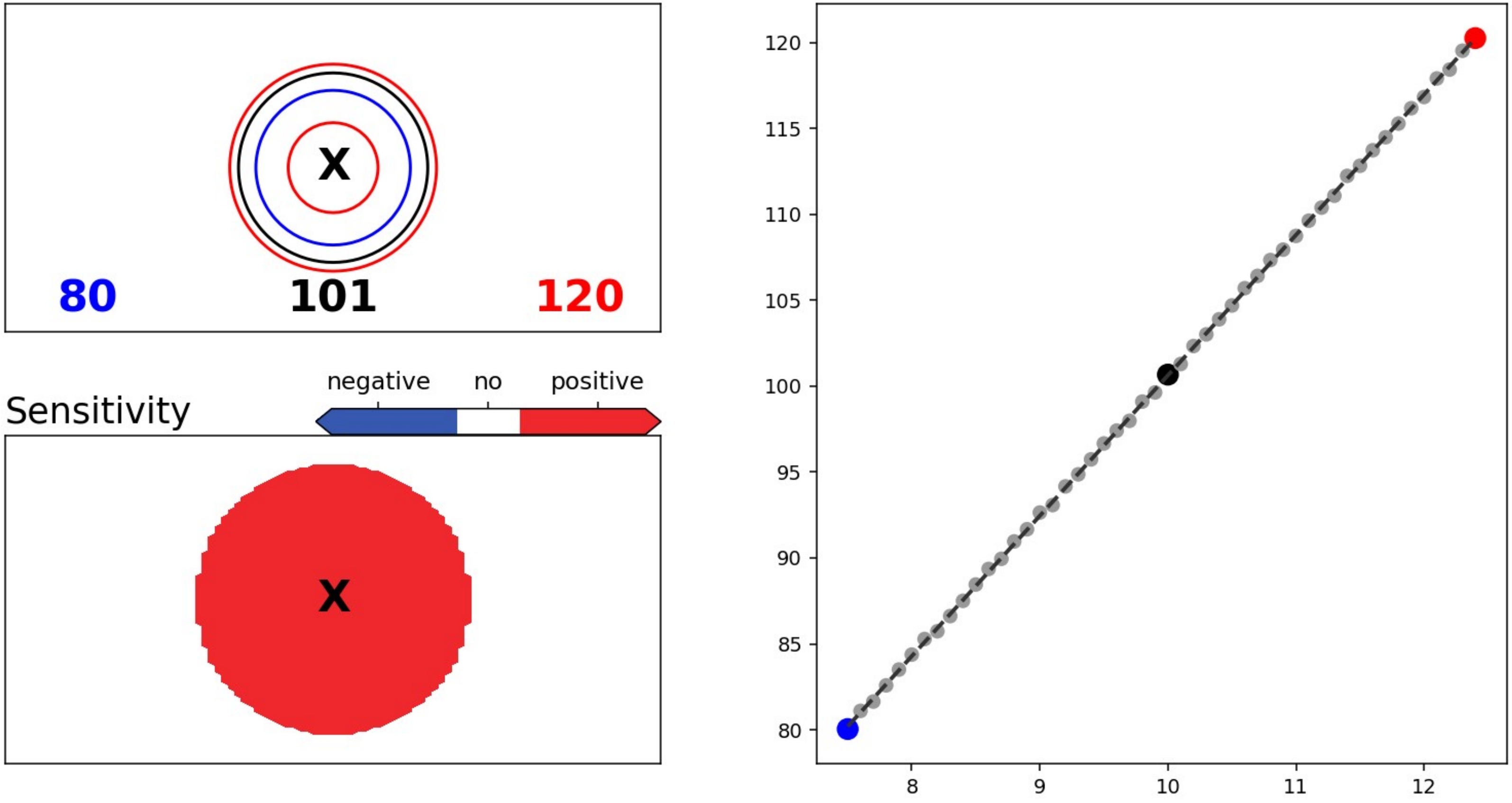
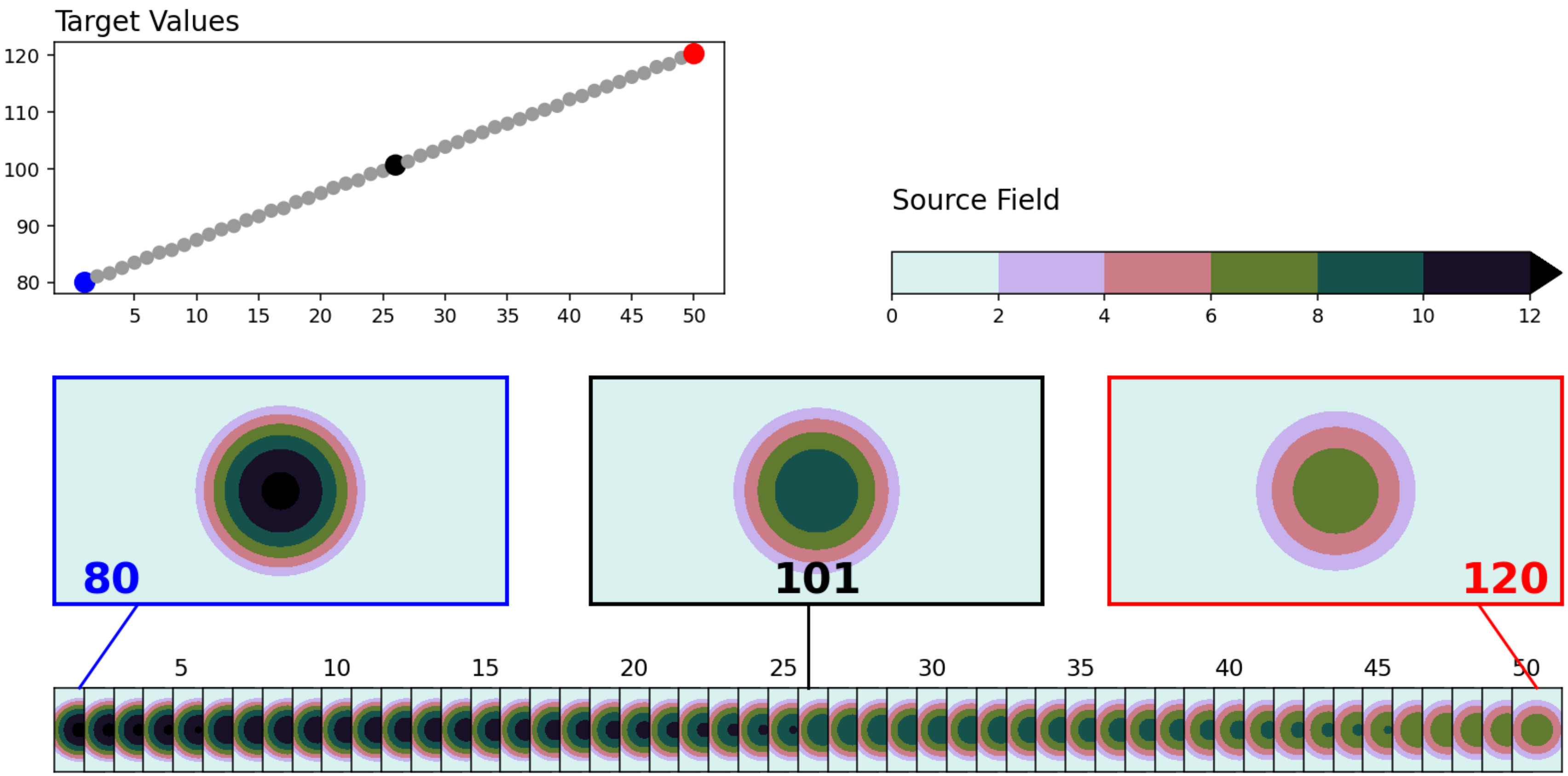


B: Blob Amplitude Uncertainty



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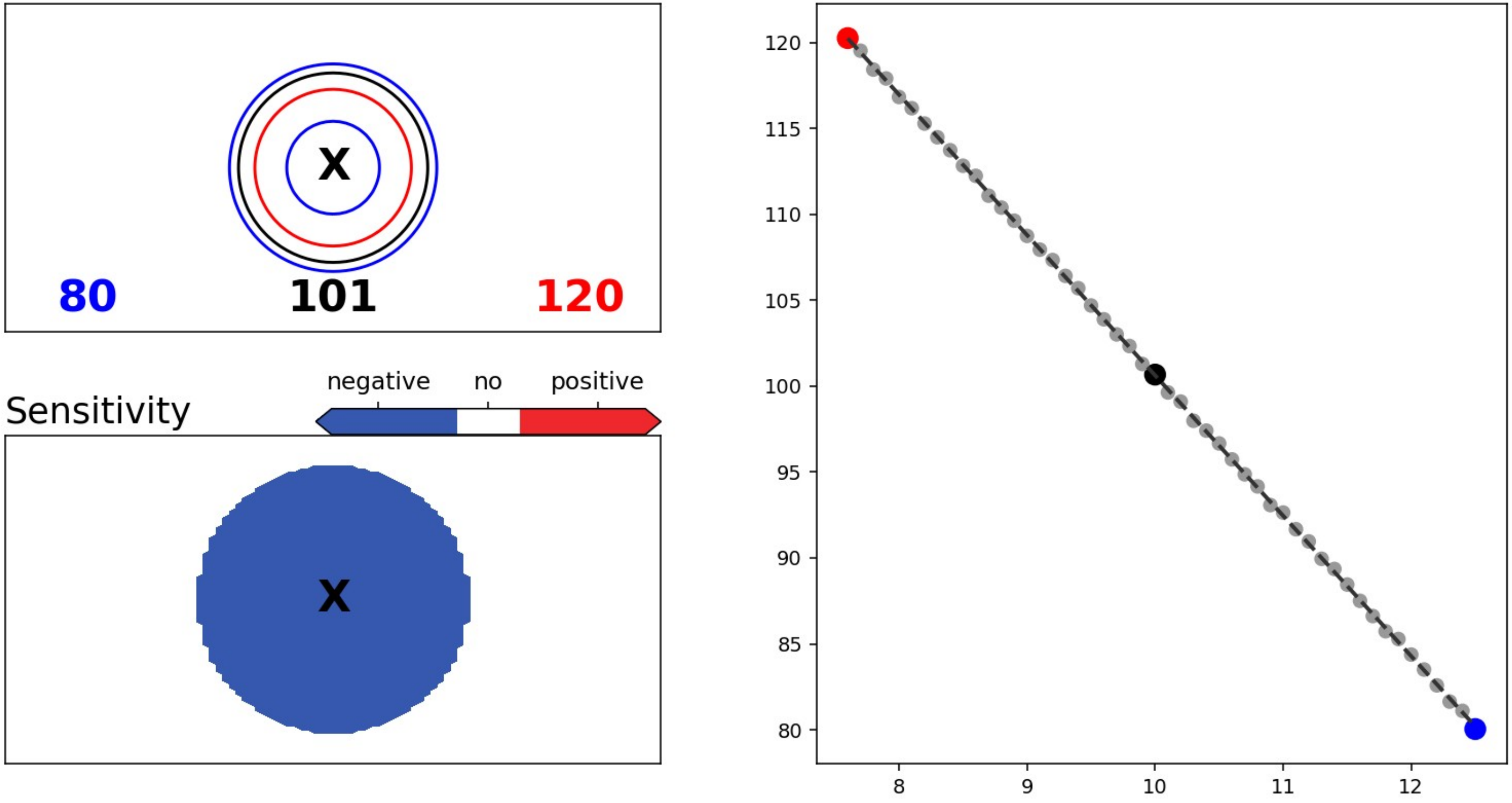
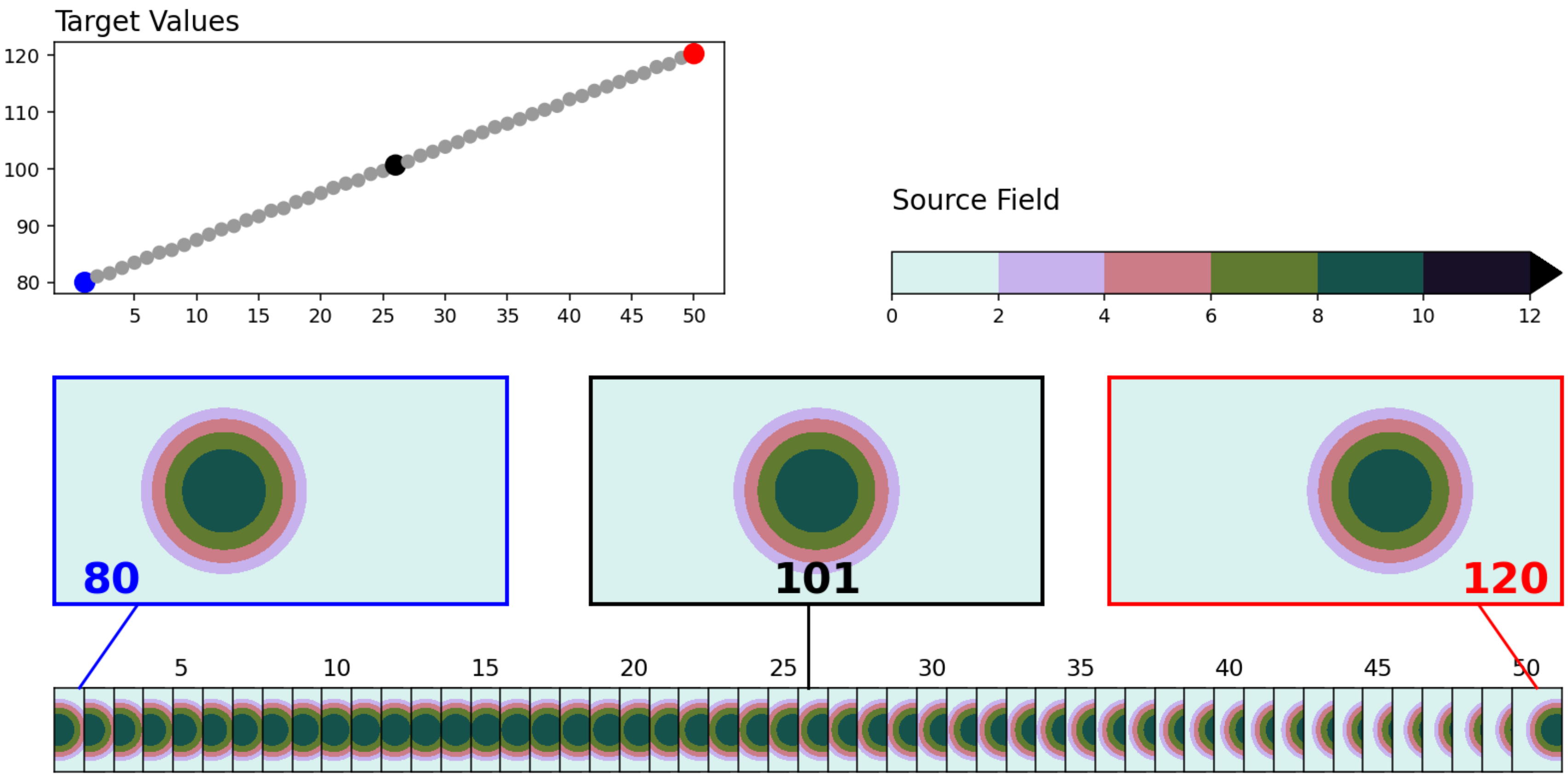


C: Blob Location Uncertainty



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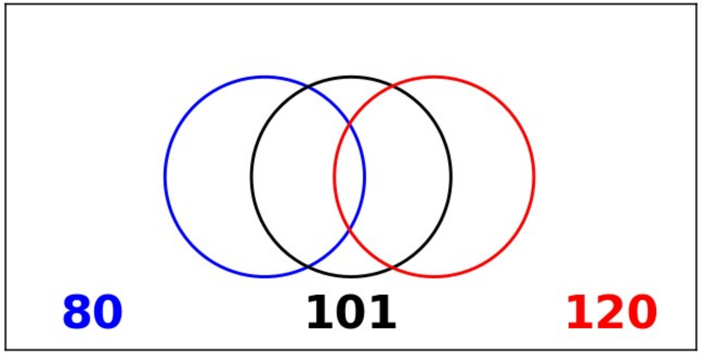

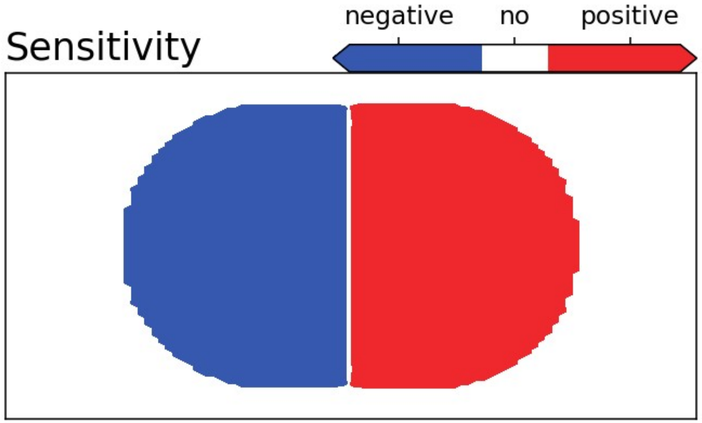

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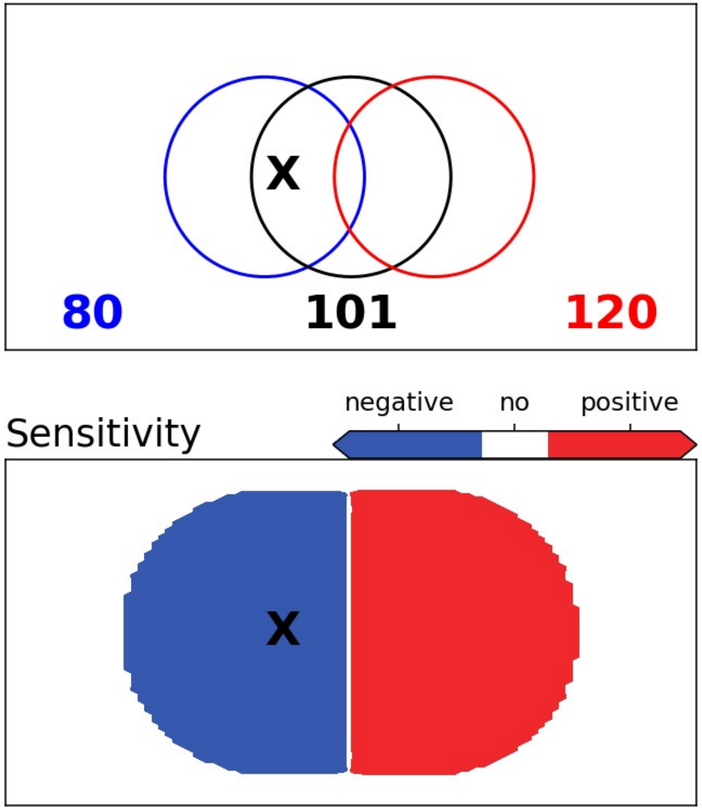

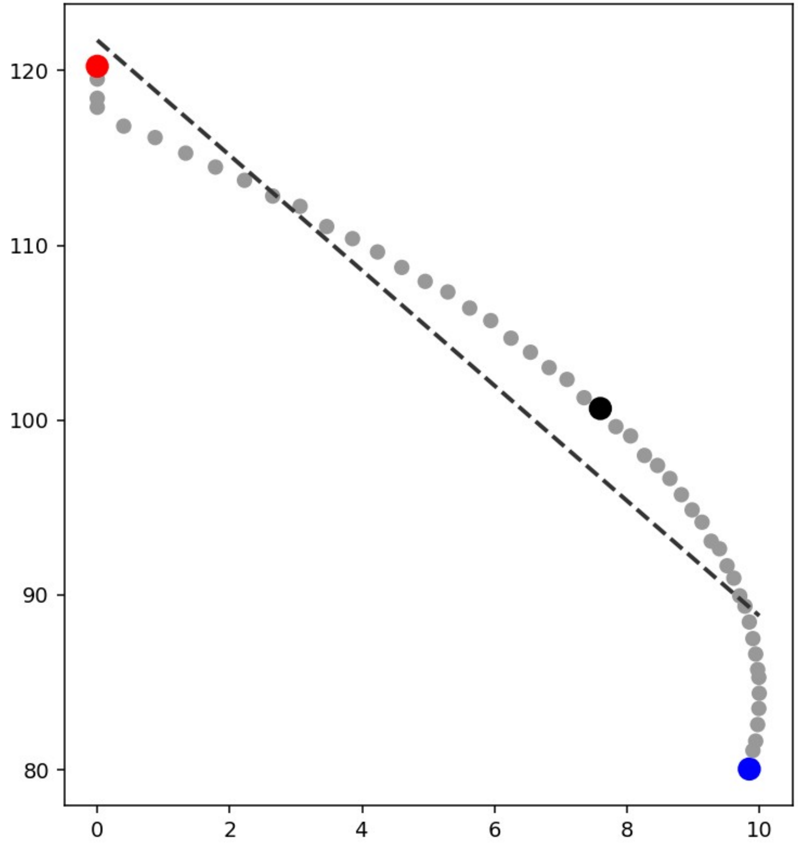

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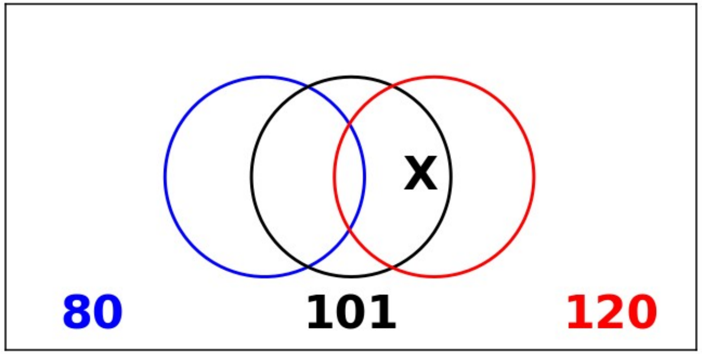

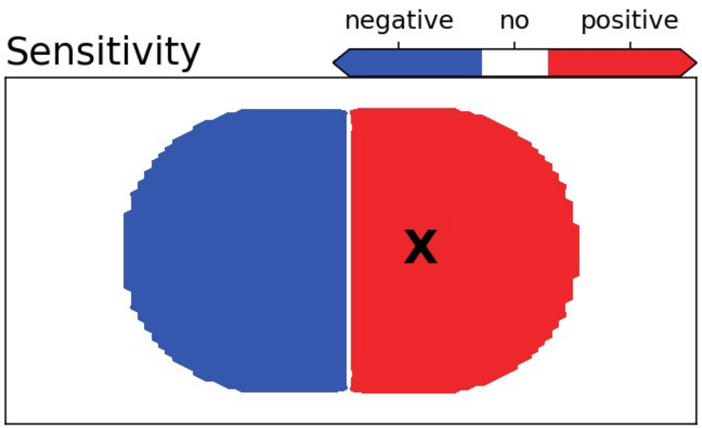

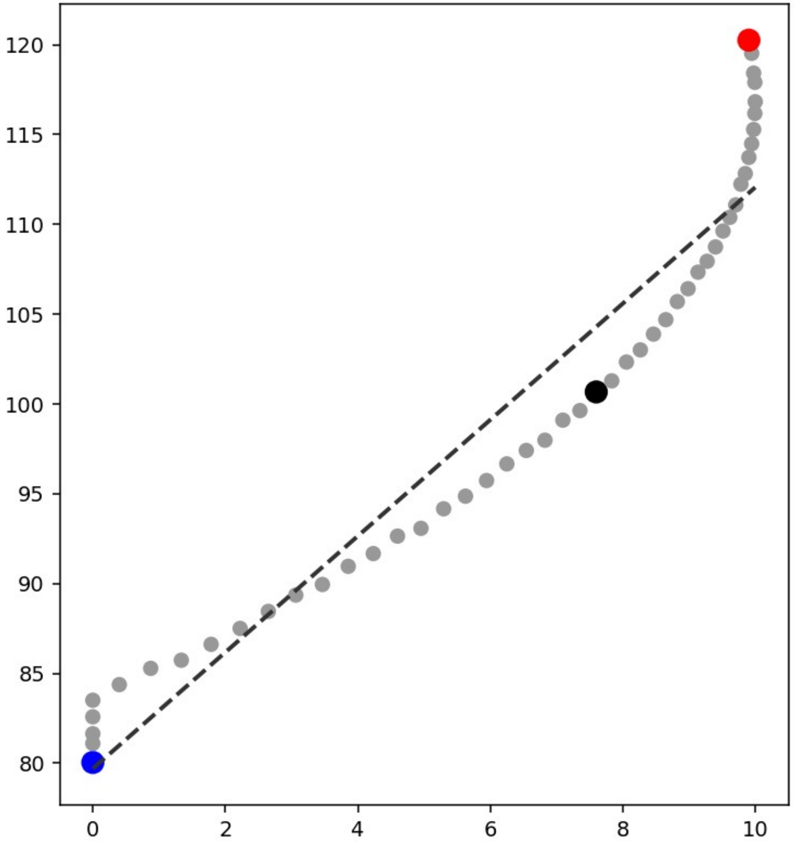

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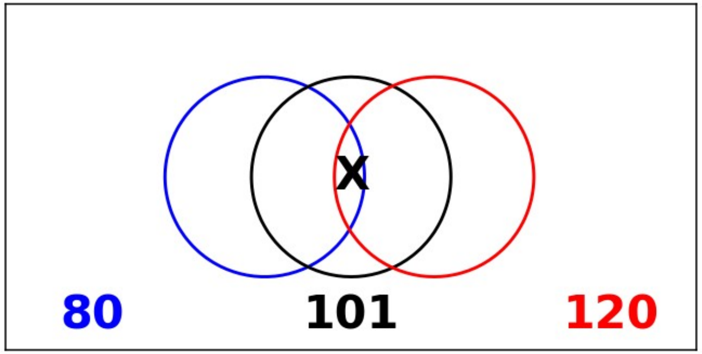
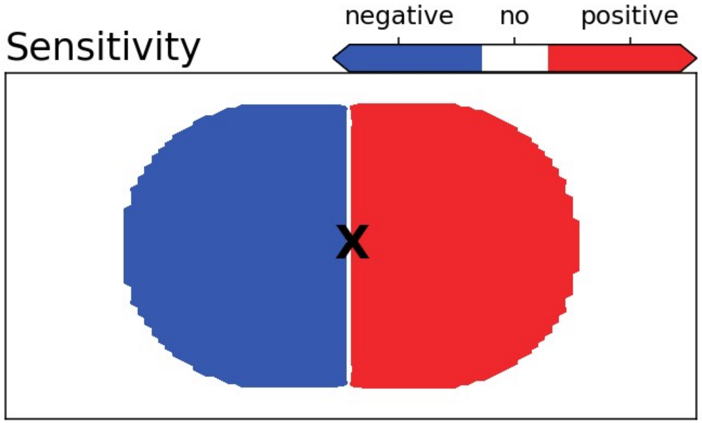
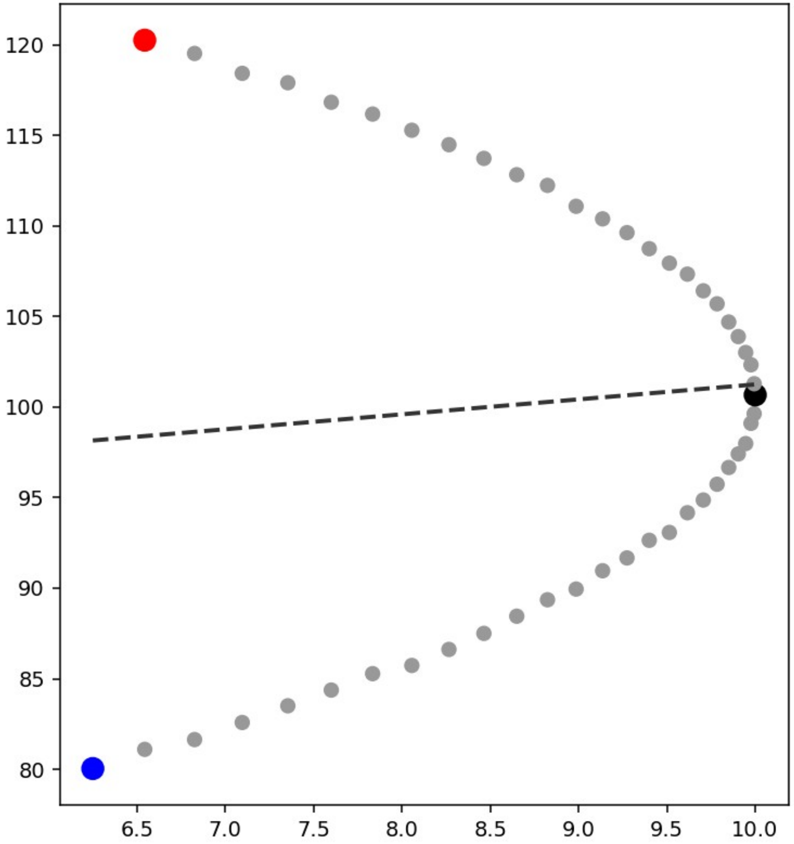
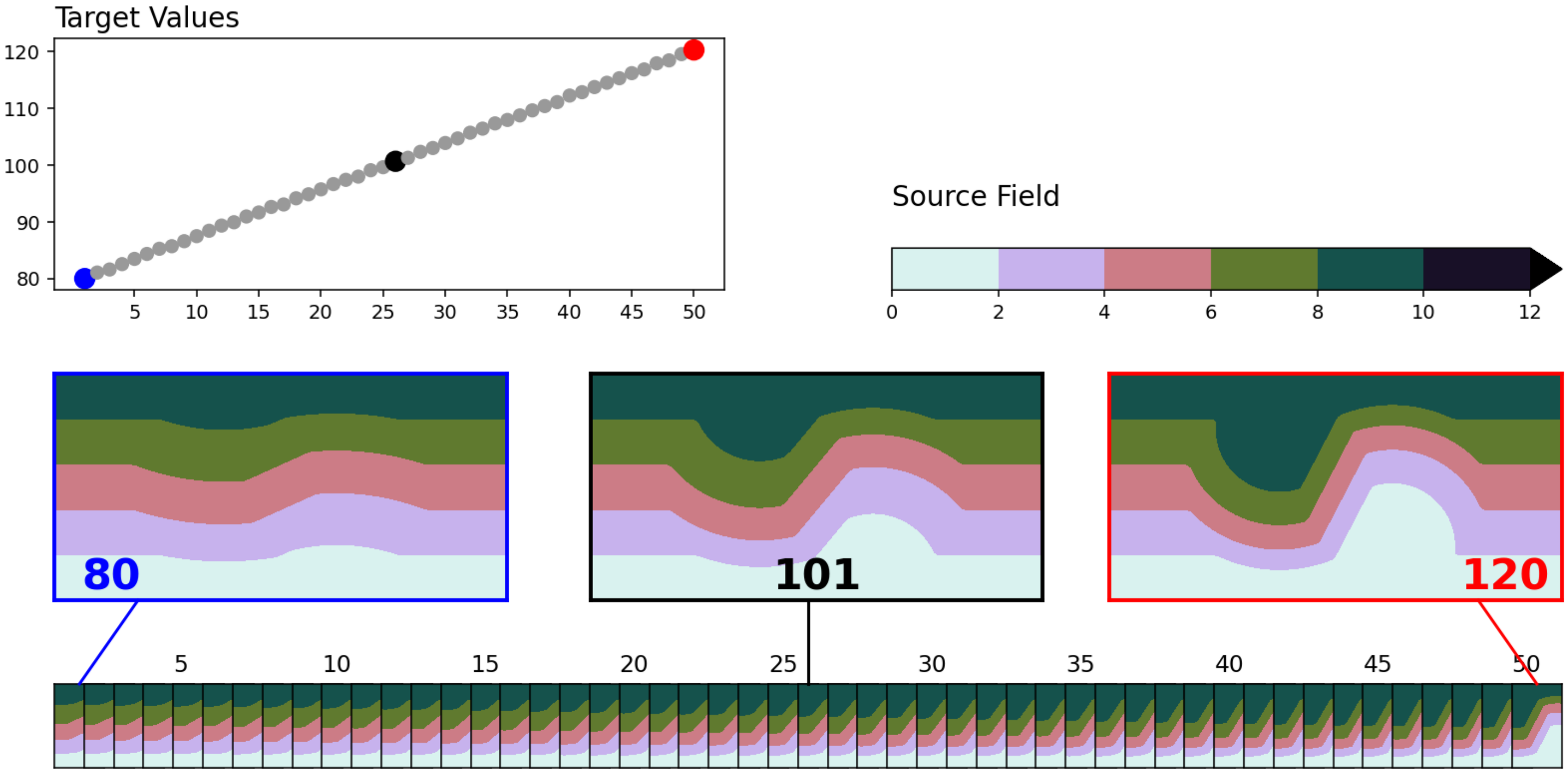






D: Wave Amplitude Uncertainty



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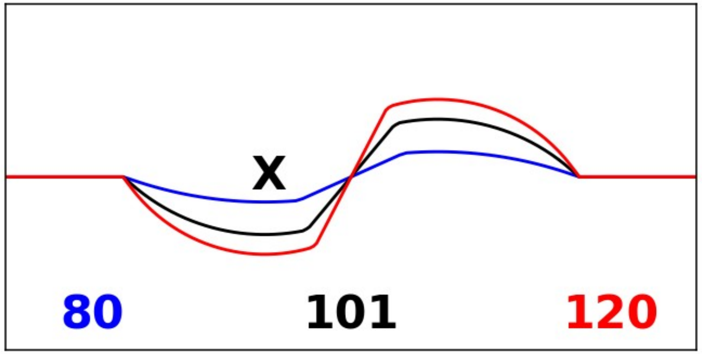
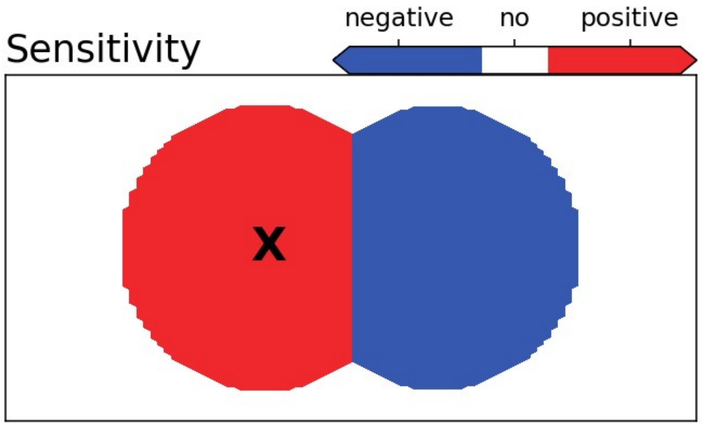
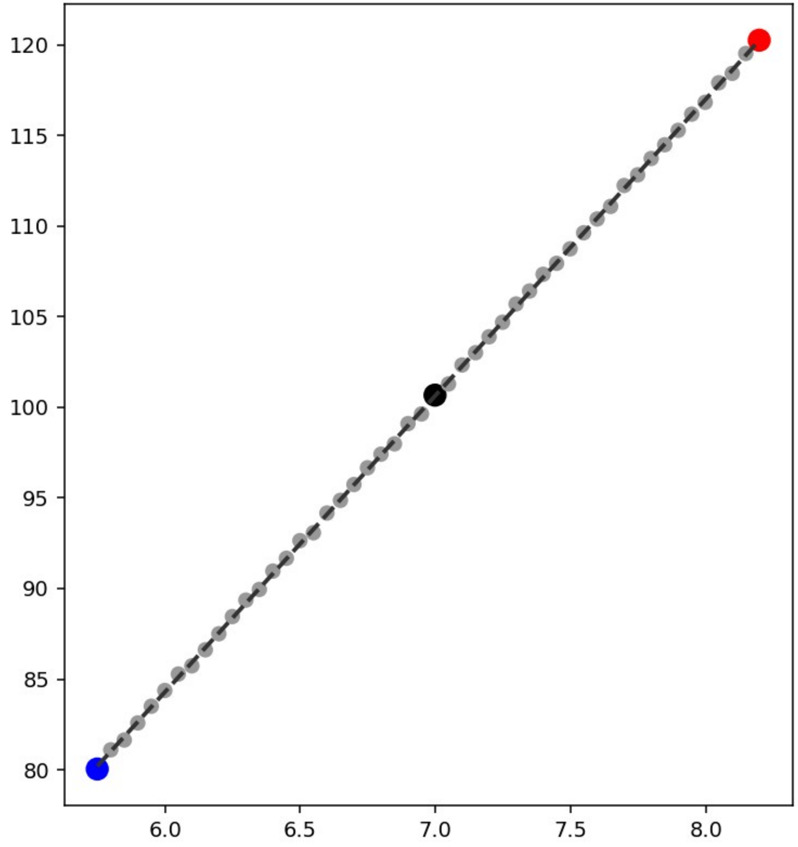
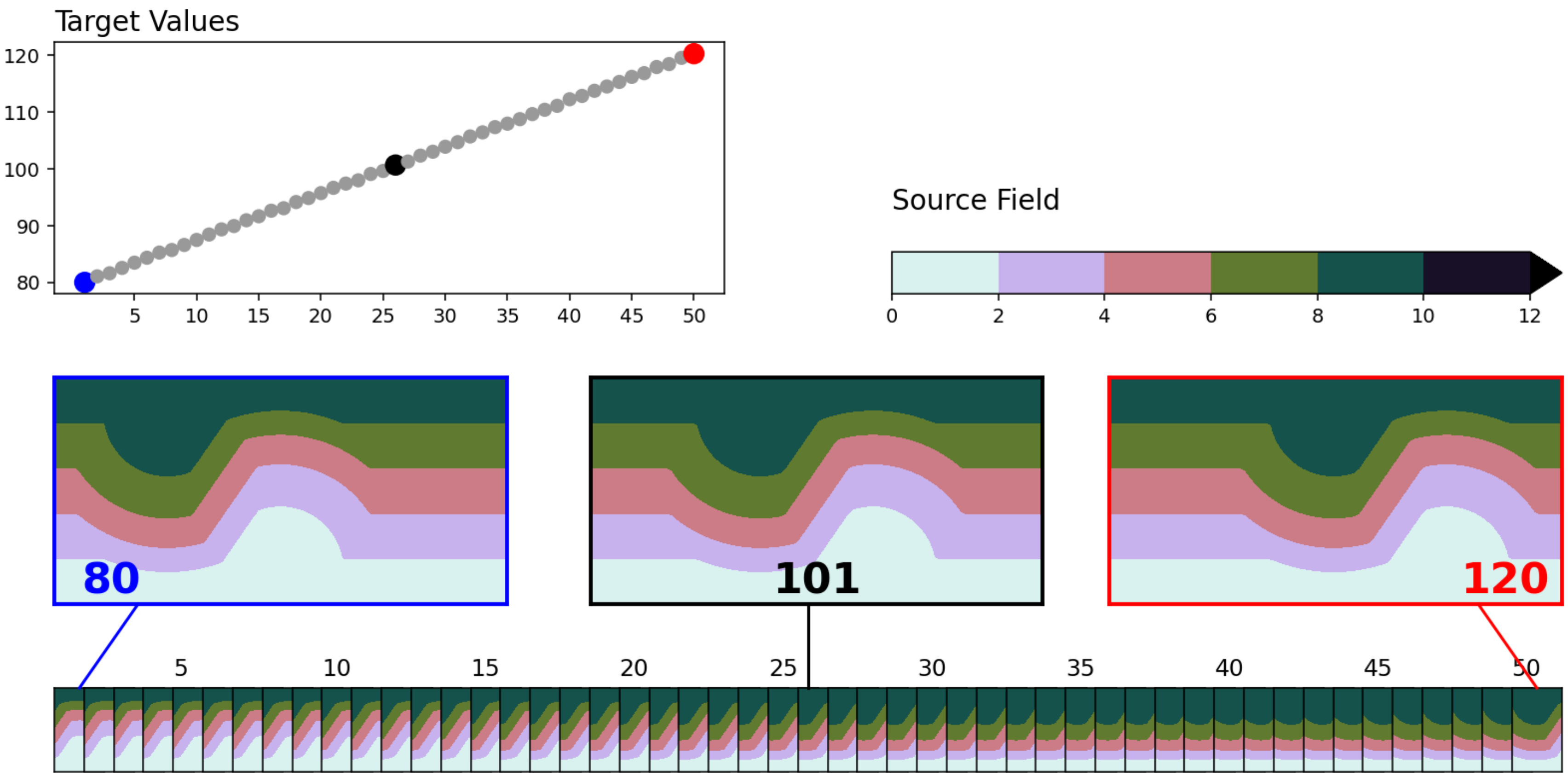






E: Wave Phase Uncertainty



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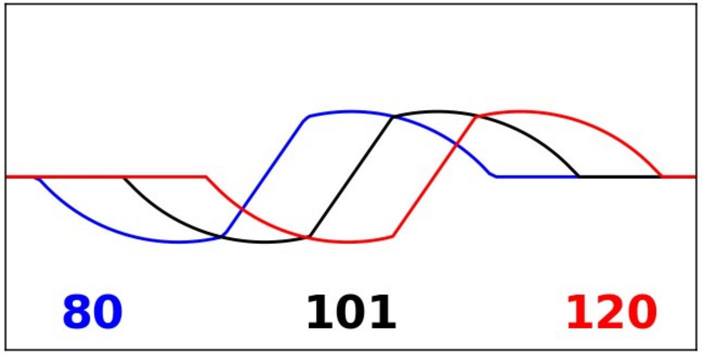

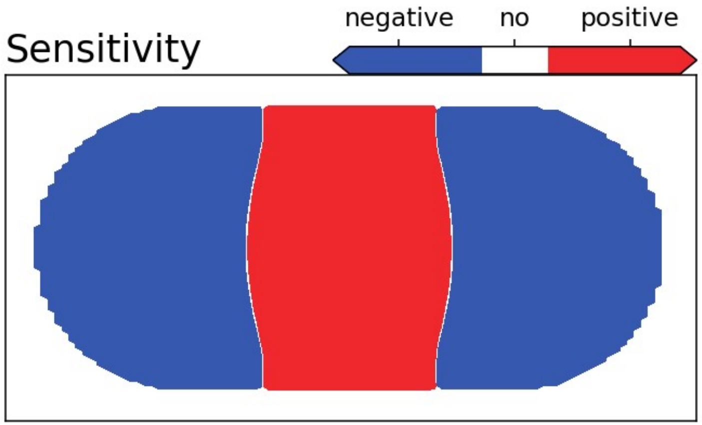

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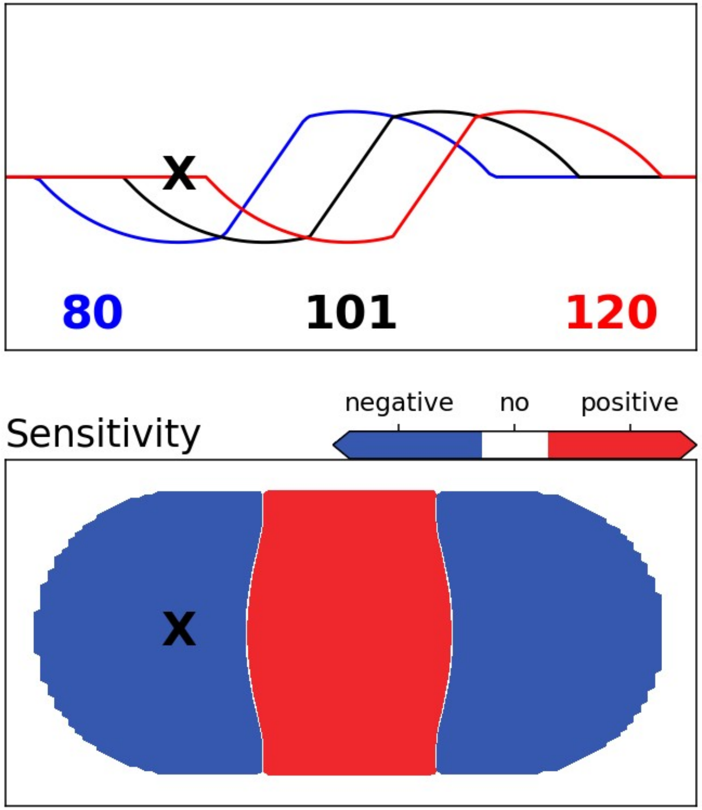

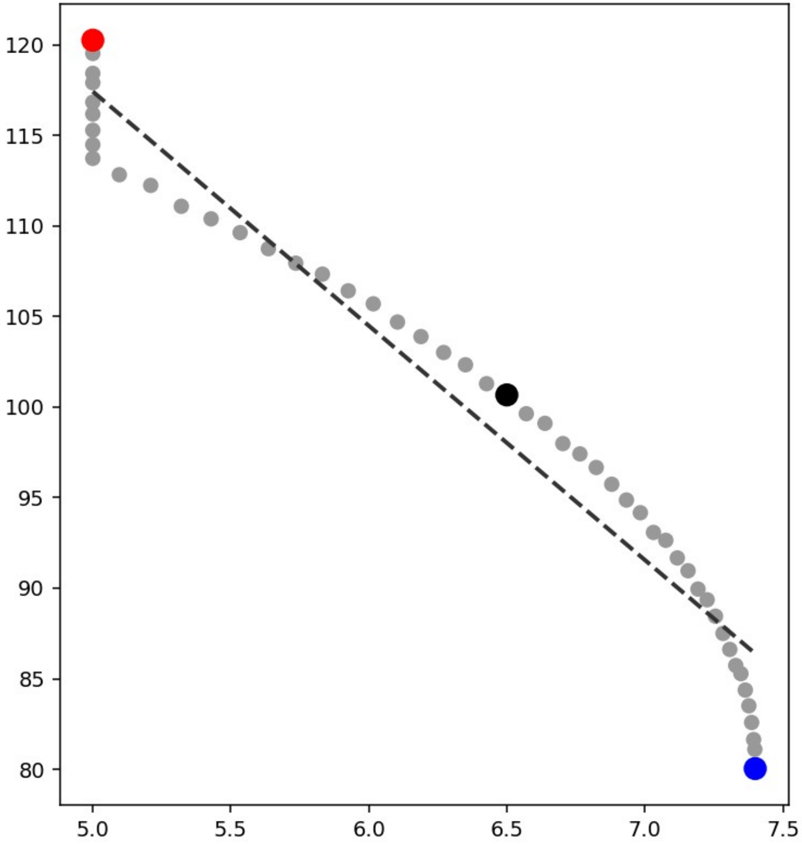

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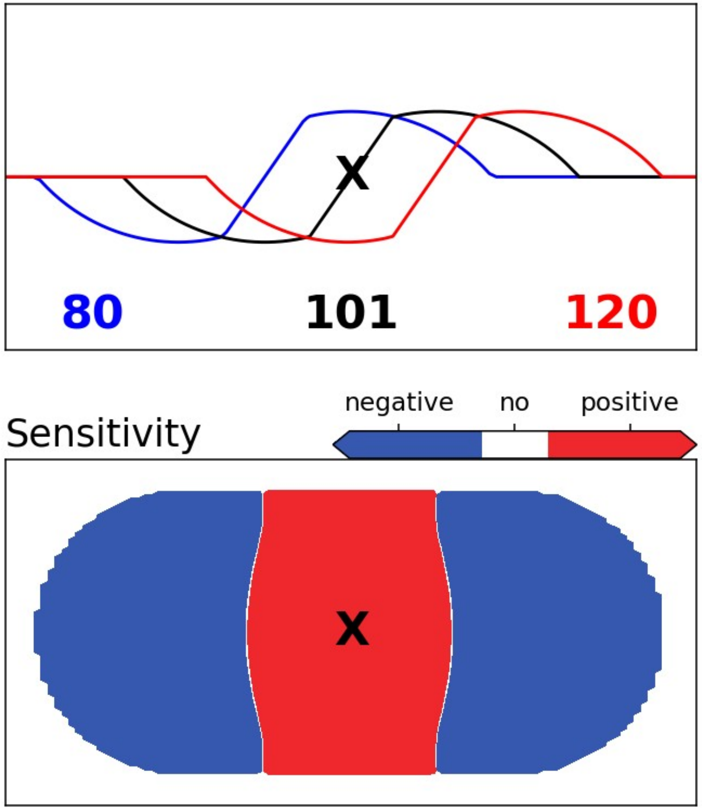

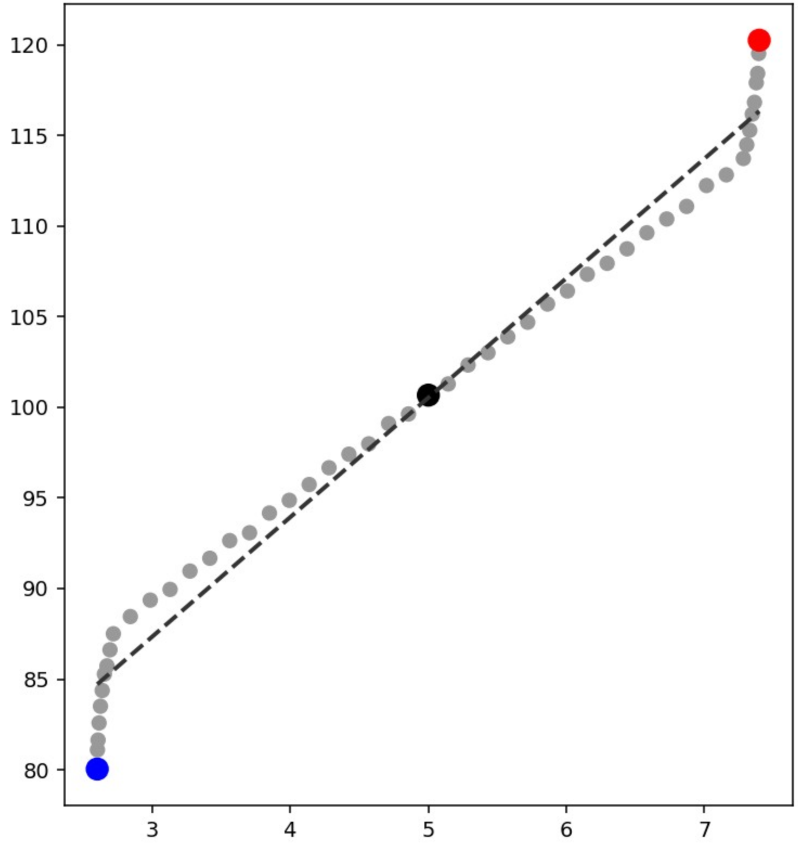

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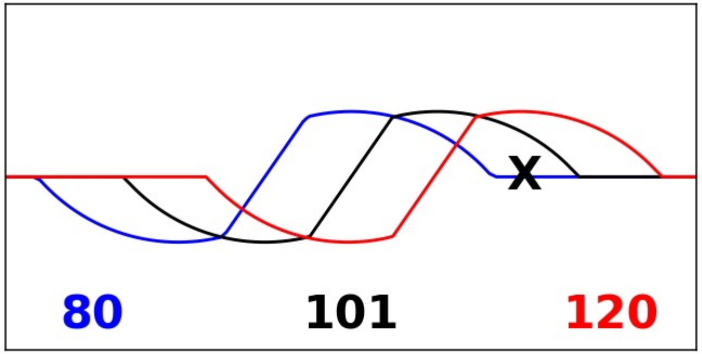
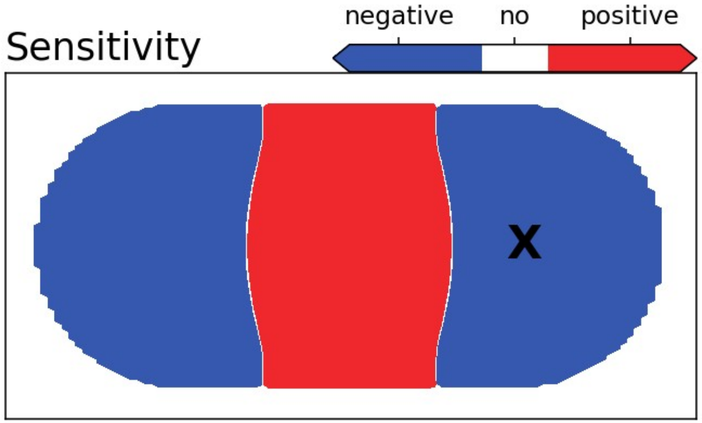
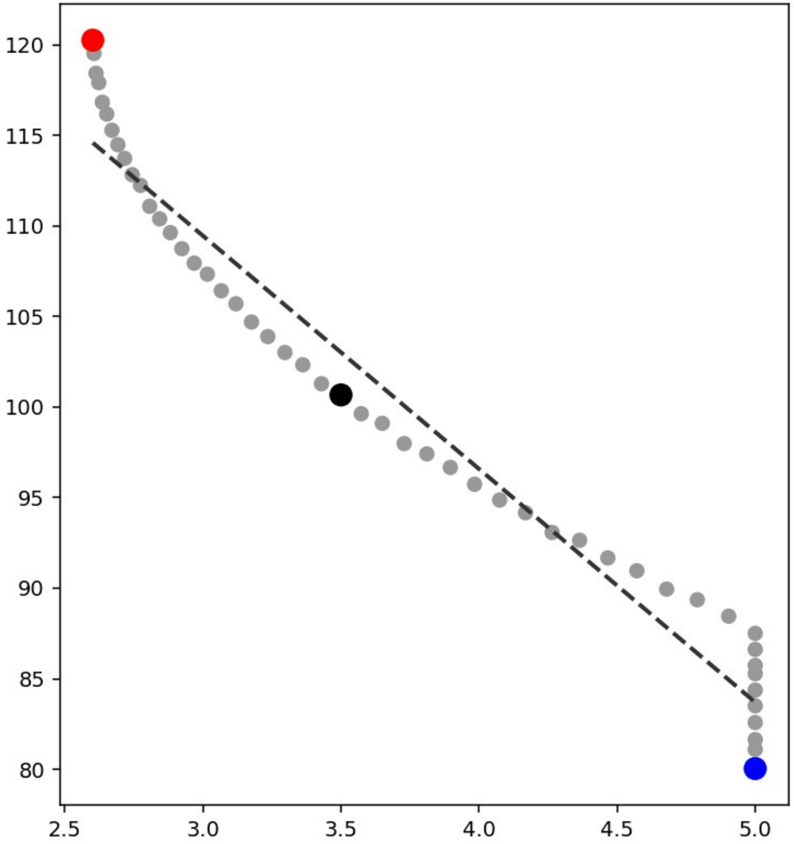






Part II

- Source fields and target metrics
- Tracking in space and time
- Causality, Limitations, Normalization
- Hands-on: ESA, Normalization

Source Fields and Target Metrics

(How (much)) does T change when S changes?

Source Field Examples:

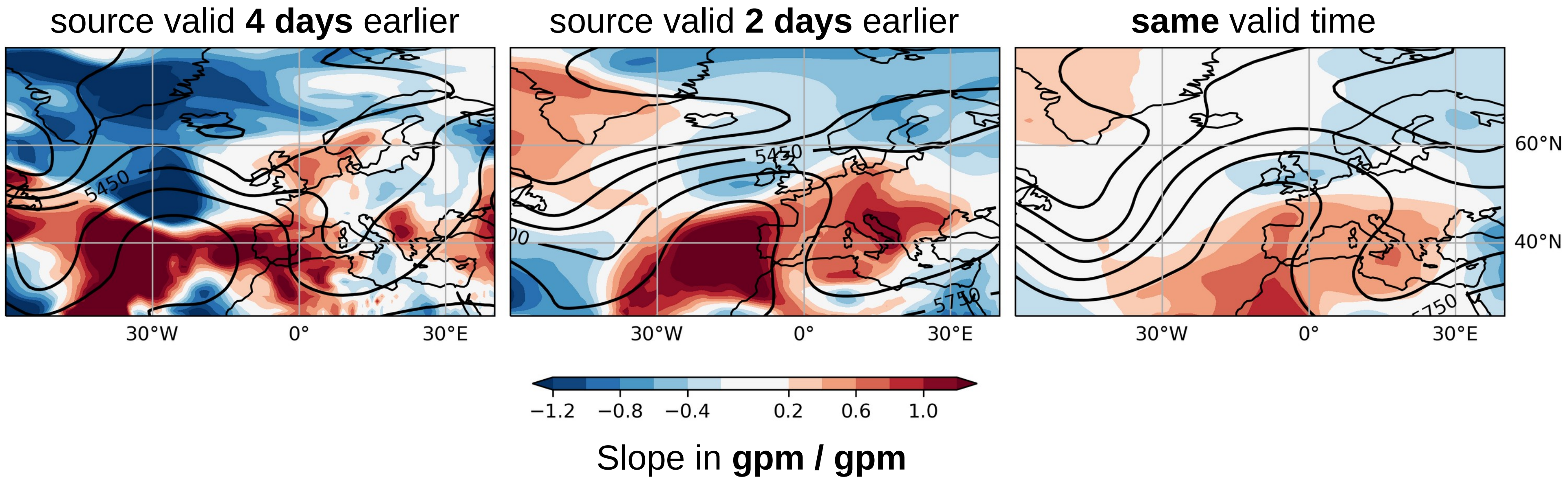
- Geopotential
- Temperature
- Moisture
- Precipitation
- Potential vorticity

Target Metric Examples:

- Forecast/Analysis Error
  - Regional RMSE, ACC, ...
- 3h-Precipitation at a location
- Cyclone central pressure
- Wind power production

Tracking in Space and Time

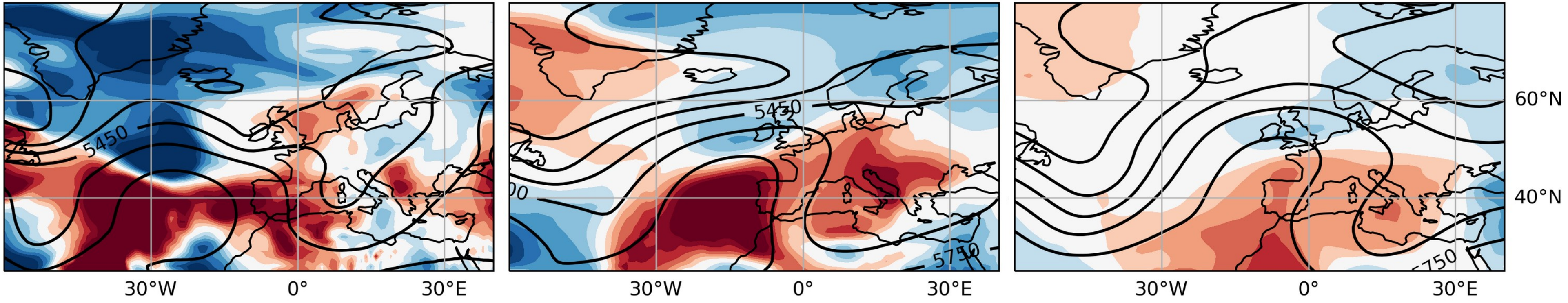
Consider source and target at **different valid times**:



Tracking in Space and Time

Consider source and target at **different valid times**:

source valid **4 days** earlier | source valid **2 days** earlier | **same** valid time



Fields are connected through evolution in model, **but**:
ESA is statistical and does **not** diagnose causality directly!

Limitations

- **Results only as good as the ensemble**
  - Garbage in, garbage out
  - Generally: bigger is better

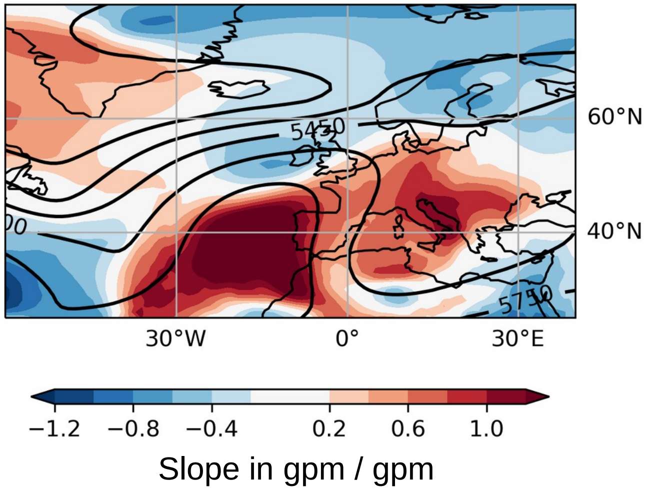
- Not all assimilation systems sample probability distribution of analysis properly
  - Throw away first timesteps to eliminate “**memory of the initial conditions**” (Hakim and Torn 2008)

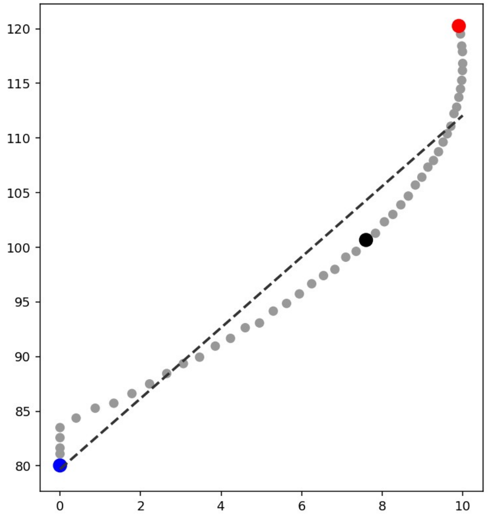
Limitations

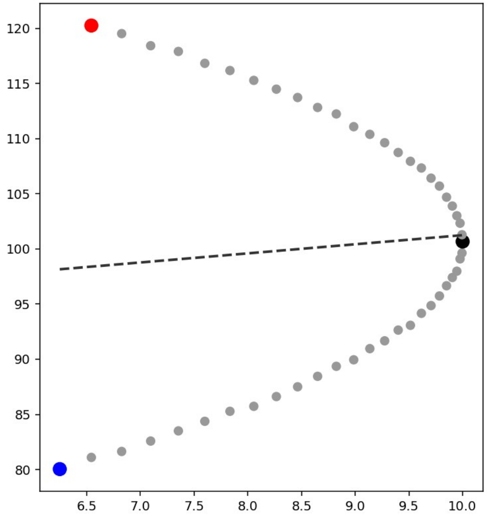
- Only **“linear” sensitivity** is measured
- **Gridpoint-wise** sensitivity, must not aggregate response

$$\mathrm{cov}\left(\boldsymbol{S},\boldsymbol{S}\right)^{-1}$$

$$\rightarrow \begin{pmatrix} \sigma_{s_1}^{-2} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_{s_m}^{-2} \end{pmatrix}$$







Normalization

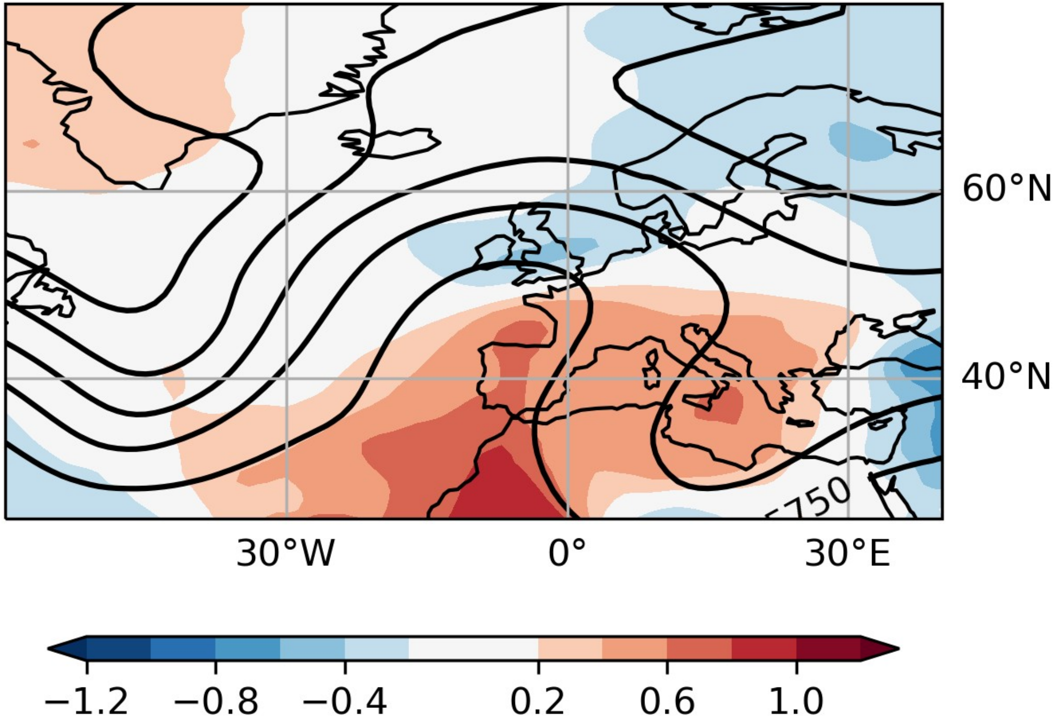
How to compare sensitivity quantitatively?

Z500 vs. Z500 Error

- Slope in gpm / **gpm**

T850 vs. Z500 Error

- Slope in gpm / **K**



Slope in **gpm / gpm**

Normalization

	No normalization of source	
No normalization of target	$$\frac{\operatorname{cov}\left(\boldsymbol{t}, \boldsymbol{s}_{\boldsymbol{i}}\right)}{\sigma_{s_i}^2}$$ slope of regression	

Normalization

	No normalization of source	Normalize source: multiply by σ_{s_i}
No normalization of target	$\dfrac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}^2}$ slope of regression	$\dfrac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}}$ compare sources

Normalization

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No normalization of target	$\dfrac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}^2}$ slope of regression	$\dfrac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}}$ compare sources
Normalize target: divide by σ_t	$\dfrac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}^2 \sigma_t}$ compare targets	

Normalization

	No normalization of source	Normalize source: multiply by σ_{s_i}
No normalization of target	$\frac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}^2}$ slope of regression	$\frac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}}$ compare sources
Normalize target: divide by σ_t	$\frac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i}^2 \sigma_t}$ compare targets	$\frac{\operatorname{cov}(\boldsymbol{t}, \boldsymbol{s_i})}{\sigma_{s_i} \sigma_t}$ correlation coefficient

Hands-on

Implement ESA
Compare Normalizations

Access to the Hands-on Material

Clone repository and run Jupyter locally:

- https://github.com/chpolste/ESA-Workshop
- Python 3 with numpy, xarray, netcdf4*, matplotlib, cartopy

Use mybinder.org and run online:

- https://mybinder.org/v2/gh/chpolste/ESA-Workshop/main
- Be aware of the 10 min inactivity timeout!

Part III

- Magnusson (2017): “Diagnostic methods ...”
- Hands-on: Tracking with ESA Maps
- Hands-on: Cluster-based Sensitivity

Magnusson (2017) Paper

Diagnostic methods for understanding the origin of forecast errors

- Investigation of 3 “forecast bust” cases
- Error tracking and confirmation with relaxation experiments

Get a copy:

- https://doi.org/10.1002/qj.3072
- https://www.ecmwf.int/en/elibrary/17097-diagnostic-methods-understanding-origin-forecast-errors

Hands-on

Tracking with ESA Maps
Cluster-based Sensitivity

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Clone repository and run Jupyter locally:

- https://github.com/chpolste/ESA-Workshop
- Python 3 with numpy, xarray, netcdf4*, matplotlib, cartopy

Use mybinder.org and run online:

- https://mybinder.org/v2/gh/chpolste/ESA-Workshop/main
- Be aware of the 10 min inactivity timeout!

References

Data

- Ensemble forecast data: ECMWF (TIGGE) https://apps.ecmwf.int/datasets/licences/tigge/
- Reanalysis data (verification): ERA5 (CDS) https://dx.doi.org/10.24381/cds.bd0915c6

Sensitivity pattern quiz inspired by Fig. 1 of Maddison et al. (2019)

Literature

- Ancell, B., & Hakim, G. J. (2007). Comparing Adjoint- and Ensemble-Sensitivity Analysis with Applications to Observation Targeting. Monthly Weather Review, 135(12), 4117–4134. https://doi.org/10.1175/2007MWR1904.1
- Gombos, D. (2009). Ensemble regression: Using ensemble model output for atmospheric dynamics and prediction [MIT]. https://dspace.mit.edu/handle/1721.1/47844
- Gombos, D., & Hansen, J. A. (2008). Potential Vorticity Regression and Its Relationship to Dynamical Piecewise Inversion. Monthly Weather Review, 136(7), 2668–2682. https://doi.org/10.1175/2007MWR2165.1
- Hakim, G. J., & Torn, R. D. (2008). Ensemble Synoptic Analysis. In L. F. Bosart & H. B. Bluestein (Eds.), Synoptic—Dynamic Meteorology and Weather Analysis and Forecasting (pp. 147–161). American Meteorological Society. https://doi.org/10.1007/978-0-933876-68-2_7
- Maddison, J. W., Gray, S. L., Martínez-Alvarado, O., & Williams, K. D. (2019). Upstream Cyclone Influence on the Predictability of Block Onsets over the Euro-Atlantic Region. Monthly Weather Review, 147(4), 1277–1296. https://doi.org/10.1175/MWR-D-18-0226.1
- Magnusson, L. (2017). Diagnostic methods for understanding the origin of forecast errors. Quarterly Journal of the Royal Meteorological Society, 143(706), 2129–2142. https://doi.org/10.1002/qj.3072