Lecture on air quality modeling:
Photostationary state of O_3 and NO_x

Gerbrand Koren Wageningen University 3 November, 2020

Learning goals for today

Learn about photostationary state between O_3 and NO_x (= NO + NO_2).

- Describe the spatial distribution of NO_2 over Europe
- Derive equations for the steady state between O_3, NO and NO_2
- Use a Jupyter Notebook to perform calculations
- Understand main features in urban measurements of NO

A short recap

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- Mixing ratios of main gases in the atmosphere (not including H_2O)

Table 1-1 Mixing ratios of gases in dry air

Gas	Mixing ratio (mol/mol)
Nitrogen (N_2)	0.78
Oxygen (O_2)	0.21
Argon (Ar)	0.0093
Carbon dioxide (CO_2)	365×10^{-6}
Neon (Ne)	18×10^{-6}
Ozone (O_3)	$0.01\text{-}10 \times 10^{-6}$

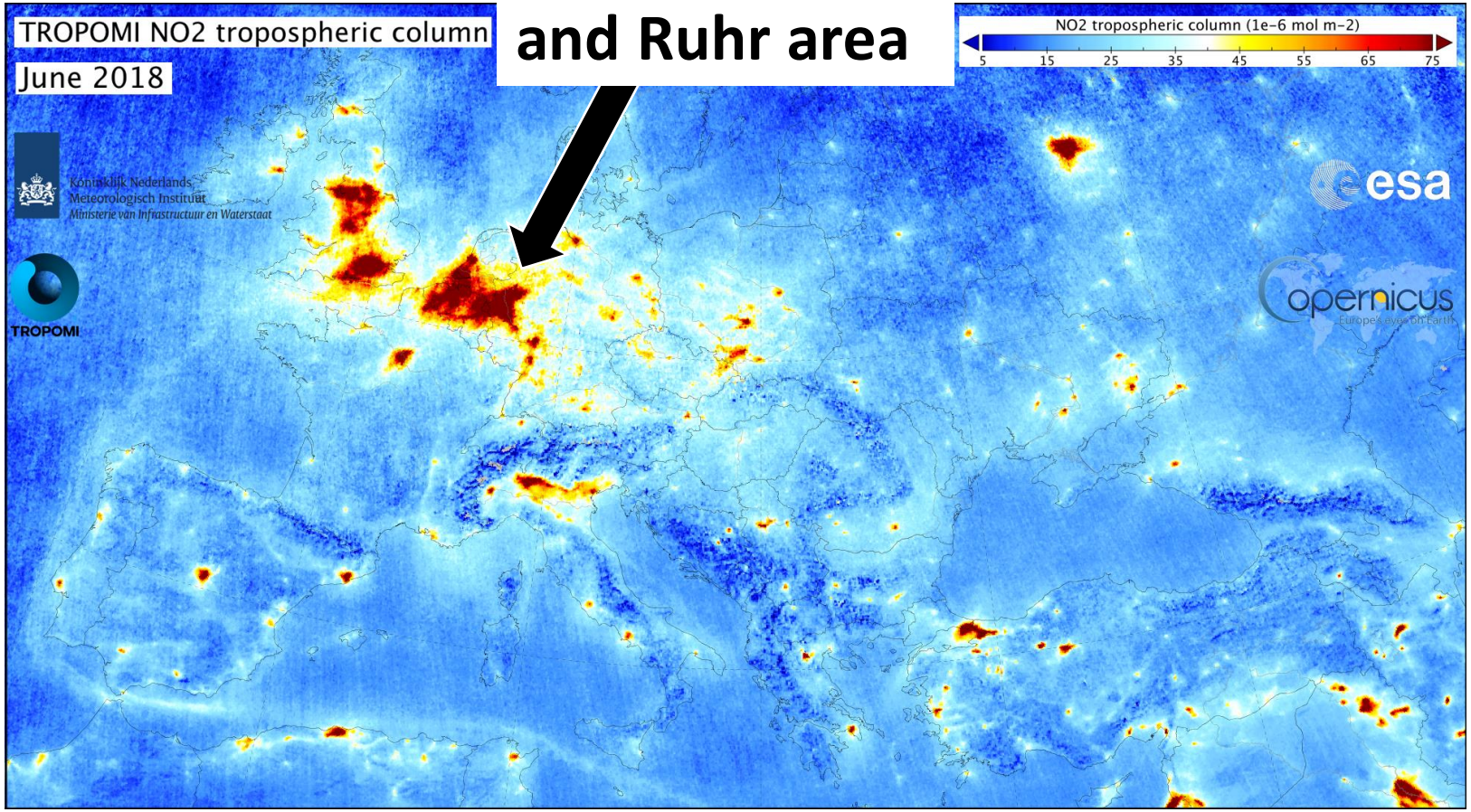
Source: Jacob (1999)

View of NO_2 from TROPOMI

- Satellites are powerful tools to study air quality
- Dutch instrument TROPOMI has a high spatial resolution
- The Netherlands is one of the hotspots for the pollutant NO_2

Netherlands and Ruhr area

Source: tropomi.eu



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- Photolysis of NO_2 requires light and produces an oxygen radical (O)

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Destruction of NO

Conversion rates

$$[\mathrm{NO}] \text{ production rate} = J_{\mathrm{NO_2}}[\mathrm{NO_2}]$$

$$\mathrm{NO_2} + h\nu \xrightarrow{J_{\mathrm{NO_2}}} \mathrm{NO} + \mathrm{O}$$

Production of NO

$$[\mathrm{NO}] \text{ destruction rate} = k_2[\mathrm{NO}][\mathrm{O_3}]$$

$$\mathrm{NO} + \mathrm{O_3} \xrightarrow{k_2} \mathrm{NO_2} + \mathrm{O_2}$$

Destruction of NO

Photostationary state

- Change in [NO] follows from the balance between production and destruction

$$\frac{d[\mathrm{NO}]}{dt} = J_{\mathrm{NO_2}}[\mathrm{NO_2}] - k_2[\mathrm{NO}][\mathrm{O_3}]$$

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$$\frac{[\mathrm{NO_2}]}{[\mathrm{NO}]} = \frac{k_2[\mathrm{O_3}]}{J_{\mathrm{NO_2}}}$$

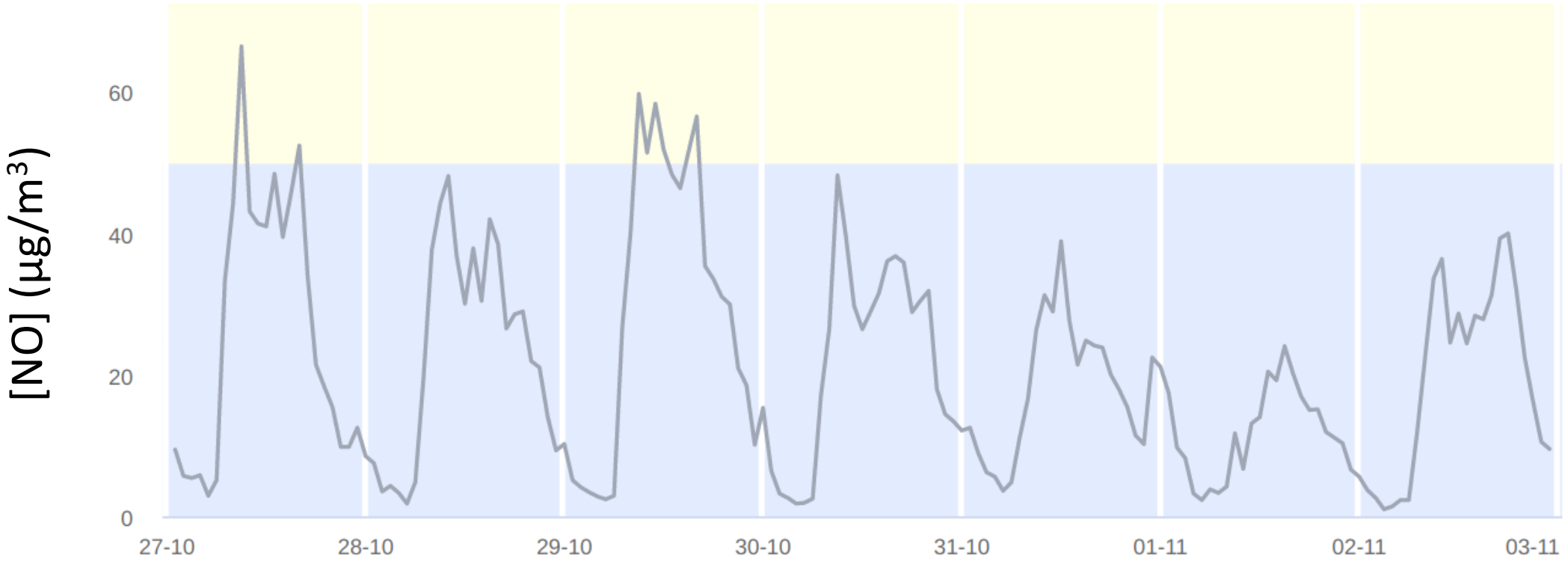
$J_{NO2} \rightarrow 0$, so $[NO_2]/[NO]$ increases rapidly, in other words NOx will be present as NO_2

Jupyter Notebook

Source: jupyter.org

- An interactive tool to write text, code and create figures with your favorite programming language!

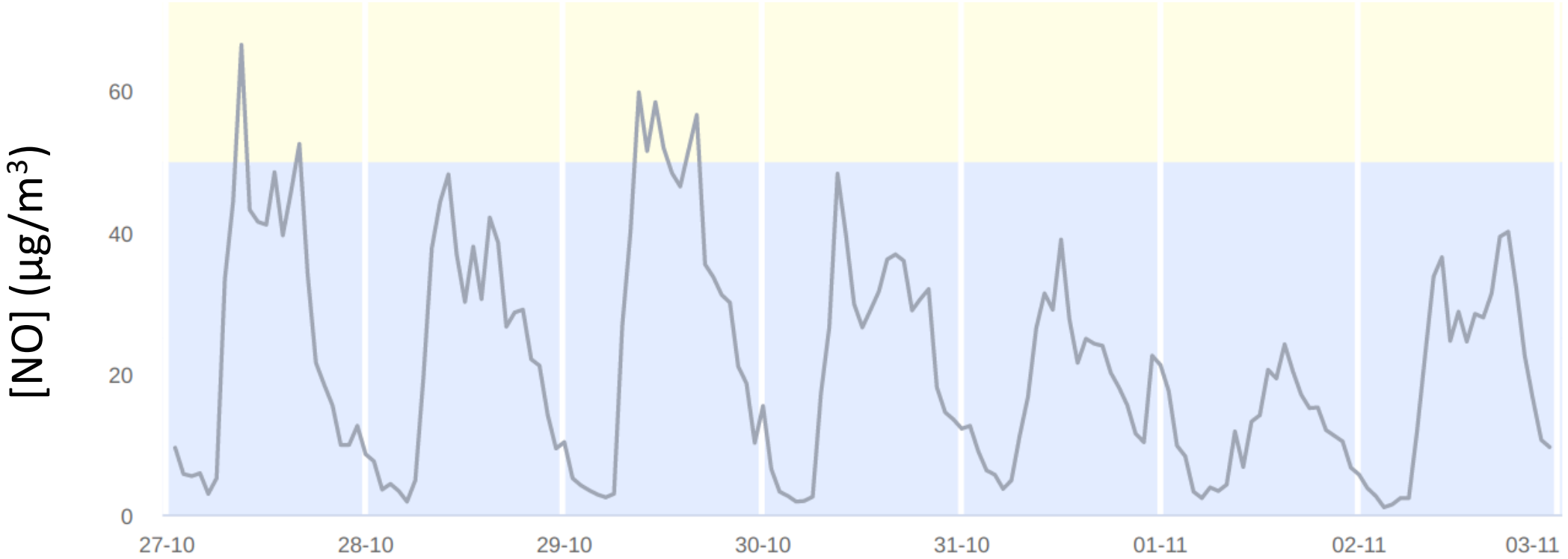
Urban air quality measurements



- Data from station Amsterdam-Haarlemmerweg for last 7 days (Luchtmeetnet.nl)

Urban air quality measurements

Q: Who can explain the measured signal?



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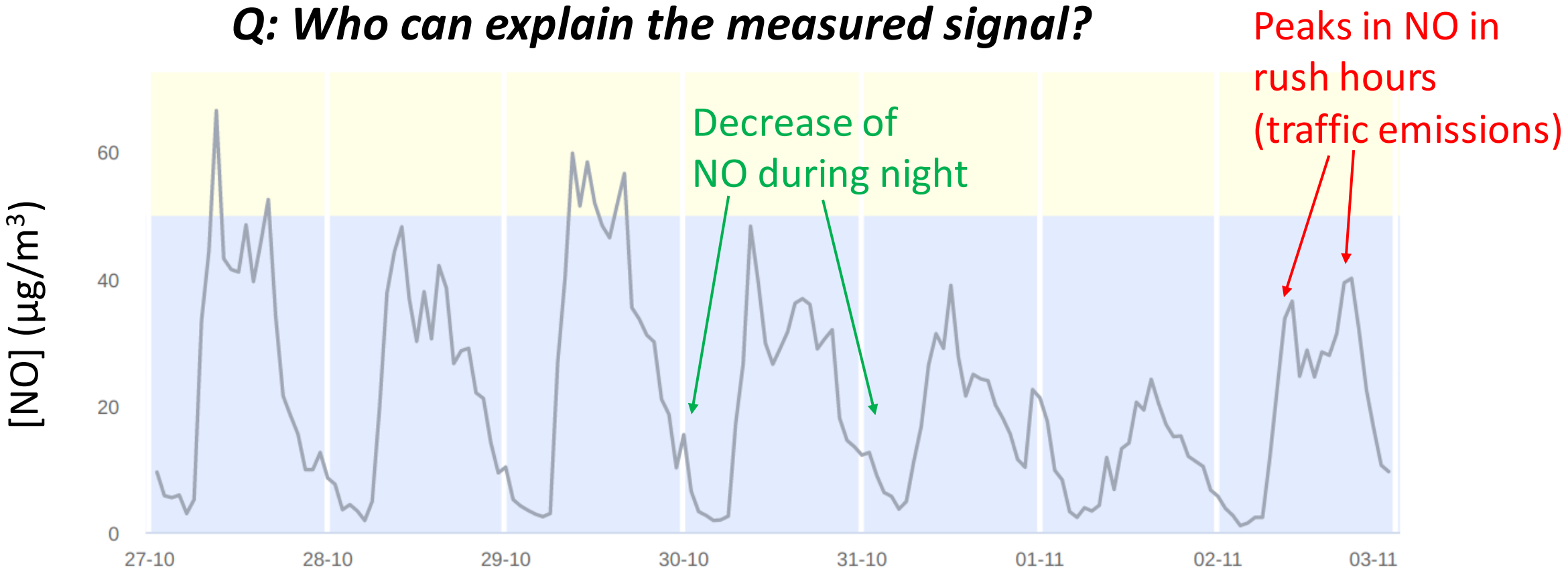

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Summary

Learned about photostationary state between O_3 and NO_x (= NO + NO_2)

- A view of NO_2 from TROPOMI: Netherlands is one of the hotspots
- Derived analytical equations for steady state between O_3, NO and NO_2
- Worked with a Jupyter Notebook to explore these equations
- Observed peaks in NO related to traffic and decreases in NO during night in a dataset with urban measurements (Luchtmeetnet.nl).

Jupyter Notebook

Start the Jupyter Notebook in one of the following ways:

- Open the Notebook through the MyBinder link:

  → https://mybinder.org/v2/gh/koren007/AQ/HEAD

  No additional software or account needed!

- Or: download the Notebook from GitHub and run locally:

  → https://www.github.com/koren007/AQ

  Requires Anaconda installation (freely available) to run the Notebook

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