In situ and actively sensed observations plus observation quality control

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Acknowledgements to ECMWF colleagues:

Lars Isaksen, Elias Holm, Saleh Abdalla, Giovanna De Chiara, Bruce Ingleby, Mike Rennie Mohamed Dahoui

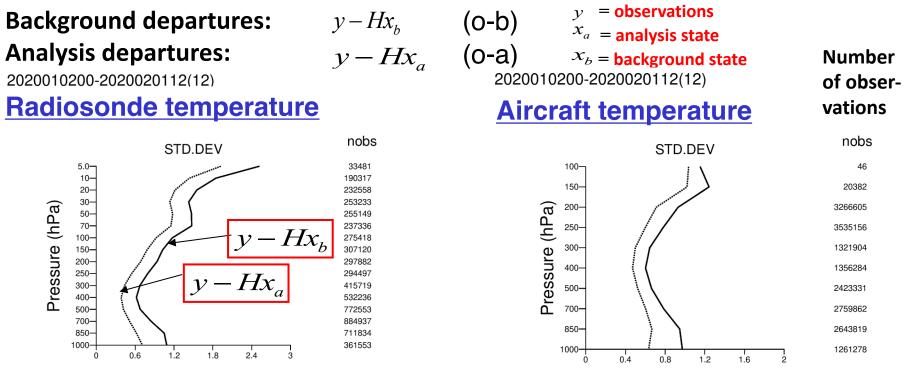
Overview of lecture

- Some jargon/definitions
- Review of in situ and actively sensed observations in global NWP
 - > How we assimilate the data, recent developments
- Quality control (briefly!)
 - What we (try to) do when the actual observation errors are not what we expect or assume, given the assumed covariance matrices R
- Broad scope for lecture. Hopefully, it will "signpost" you to useful material

Useful data assimilation jargon

- The forecast model provides the background (or *a prior*) information to the analysis
- Observation operators, *H*, enable observations and model background to be compared in "observation space"
- The differences are called departures or innovations "o-b"
 - They are central in providing observation information to the analysis
- These corrections, or increments, are added to the background to give the analysis (or *posterior estimate*)
- Observation operators also enable comparison of observations and the analysis (analysis departures "o-a")
- We'd expect abs(o-a)<abs(o-b) if the DA system is working correctly

Example: Statistics of departures

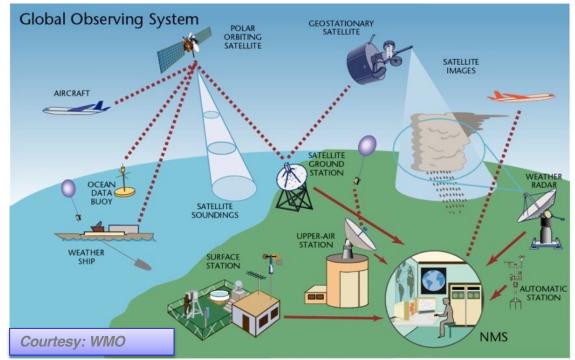


• The standard deviation of background departures for both radiosondes and aircraft is

around 0.7-1.0 K in the mid-troposphere.

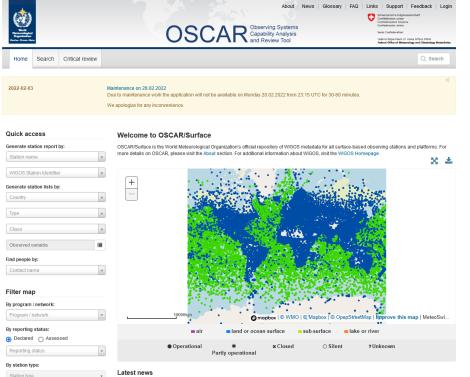
• The standard deviation of the analysis departures is smaller – because the analysis has "drawn" to the observations.

WMO Integrated Global Observing System The WMO OSCAR database provides an excellent overview



https://oscar.wmo.int/surface//index.html#/ https://www.wmo-sat.info/oscar/

WMO OSCAR (Observing Systems Capability Analysis and Review Tool)



https://oscar.wmo.int/surface//index.html#/ https://www.wmo-sat.info/oscar/

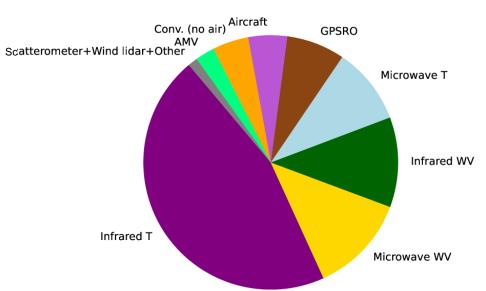
In-Situ

- Sometimes called "conventional"
- Been used since the very early days of NWP (1950's). Now about 10 % of data we use
- Providing both surface and upper-air information. Most abundant in the NH
- Usually characterized by *relatively simple* forward operators, *H*, because the measured quantities are geophysical (eg, P, T, u, v, Q). Simple, often "messy", but really still important!
- Also useful for forecast verification and help they constrain bias corrections applied to satellite radiances

• See recent fantastic review

 Pauley P, Ingleby B (2021) Assimilation of in-situ observations. In: Park SK, Xu L (eds) Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications (Vol. IV). Springer. Pages 293-371 in https://link.springer.com/book/10.1007/978-3-030-77722-7

In-situ are roughly 10 % of the data we currently assimilate - **but they have a big impact**



ops 1-Apr-2023 to 30-Apr-2023

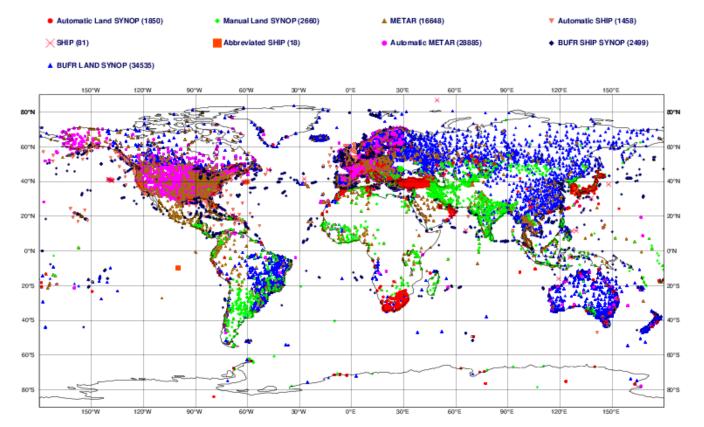
In situ data: which parameters are assimilated in atmosphere analysis?

Instrument	Parameters	Height
SYNOP SHIP METAR	pressure, dew-point temperature pressure, wind pressure	Station altitude, 2m Ships ~25m Station altitude
BUOYS	pressure, wind	MSL, 2-10m
TEMP TEMPSHIP DROPSONDES	temperature, humidity, wind	Profiles
PROFILERS	wind	Profiles
Aircraft	temperature, wind, humidity	Profiles near airports + Flight level data

Example of 6-hour SYNOP, SHIP and METAR data coverage

ECMWF data coverage (used observations) - SYNOP-SHIP-METAR 2023051821 to 2023051903

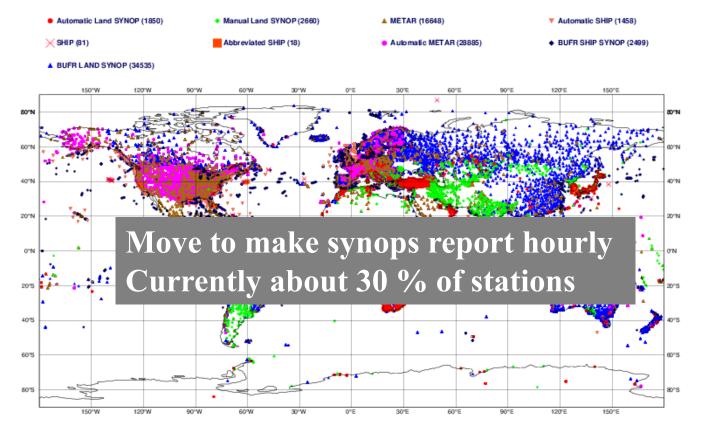
Total number of obs = 88634



Example of 6-hour SYNOP, SHIP and METAR data coverage

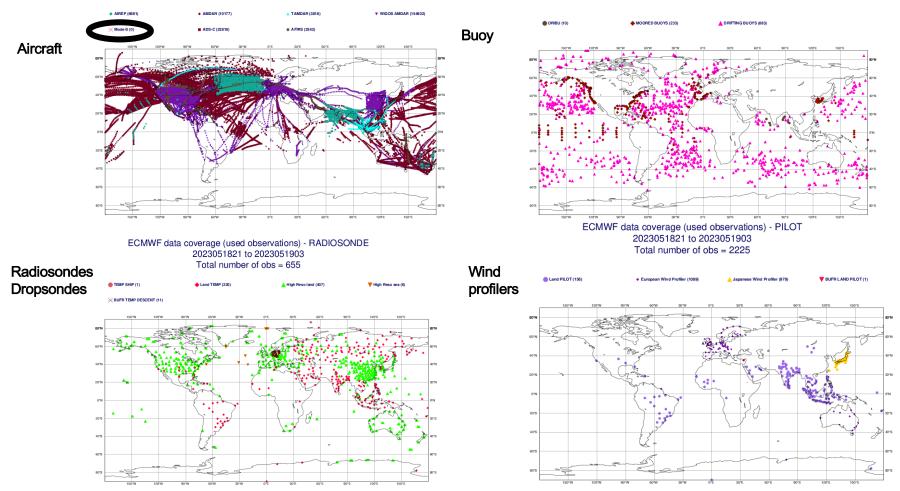
ECMWF data coverage (used observations) - SYNOP-SHIP-METAR 2023051821 to 2023051903

Total number of obs = 88634



ECMWF data coverage (used observations) - AIRCRAFT 2023051821 to 2023051903 Total number of obs = 200676

ECMWF data coverage (used observations) - BUOY 2023051821 to 2023051903 Total number of obs = 1126



Impact of various observing systems at ECMWF

Provided by Niels Bormann – 2021 annual seminar

https://events.ecmwf.int/event/217/contributions/2049/attachments/ 1397/2509/AS2021_Bormann.pdf

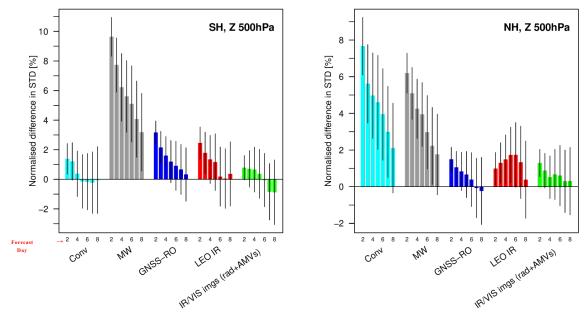


Observing system experiments – denying observation datasets

- Periods, 6 months in total: 5 Sept – 2 Nov 2020 1 Jan – 28 Feb 2021 1 May – 30 June 2021 (each + 4 days spin-up prior)
- Denial experiments compared to a full system for:
 - Conventional in-situ observations
 - MW radiances
 - IR sounders from LEO
 - IR/VIS imagers (AMVs + IR radiances)
 - GNSS-RO
- Resolution: T_{CO} 399 (~25 km)
- Background error from operational system



Forecast impact, day 2-8: 500 hPa geopotential

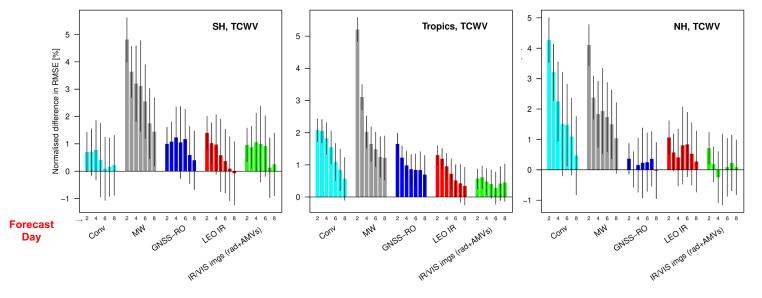


Verified against operational analyses, 3 periods combined



Forecast impact, day 2-8: Total column water vapour

Verified against operational analyses, 3 periods combined





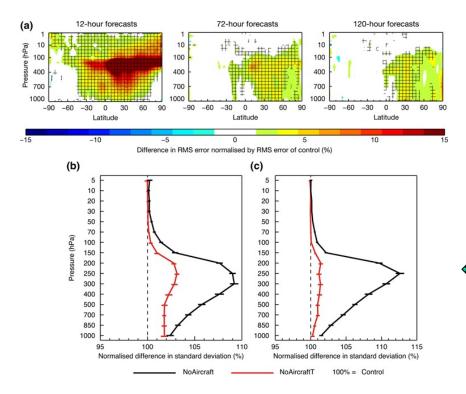
Forecast impact, day 2-8: Wind at 850 hPa

SH, VW 850hPa Tropics, VW 850hPa NH, VW 850hPa 6 6 Normalised difference in RMSE [%] 3 4 2 2 0 0 -2 2 4 6 8 LEOIR 2 4 6 8 LEOIR → 2 4 6 8 RNIS ings (ad+AM)S) 2 4 6 8 2 4 6 8 2 RNS ings (ad+AM^{S)} 2468 2 4 6 2 4 6 8 2 4 6 2 2 4 6 8 4 6 8 8 2 4 6 RIVIS ings (adriands) 2 4 6 8 Forecast GNSS-RO 55-RO ,55-RO MA M Conv MA COUN Coun Day

Verified against operational analyses, 3 periods combined



Aircraft measurements of wind more important that Temp



The short-range forecast fit to radiosondes degrades (>10% == HUGE)

b) TEMP c) wind vectors

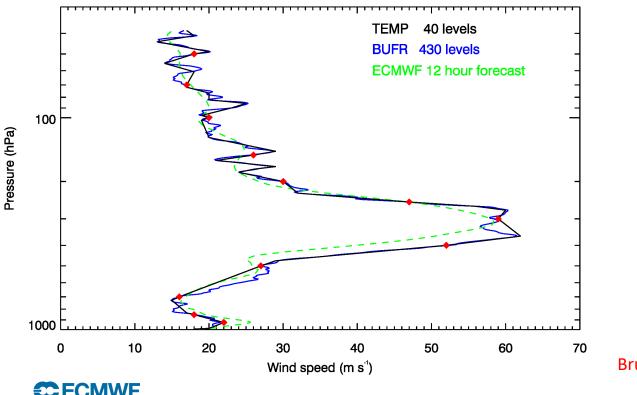
The aircraft winds provide more information than the aircraft temperatures

Geophysical Research Letters, Volume: 48, Issue: 4, First published: 06 December 2020, DOI: (10.1029/2020GL090699)

We can still improve the use of "old style" observations, like radiosonde data:

BUFR radiosondes provide up to 8000 levels of measurements compared to less than 100 levels for TAC TEMP reports. A valuable improvement for data assimilation.

ASEU04 ascent 2014 11 15 1039 UTC



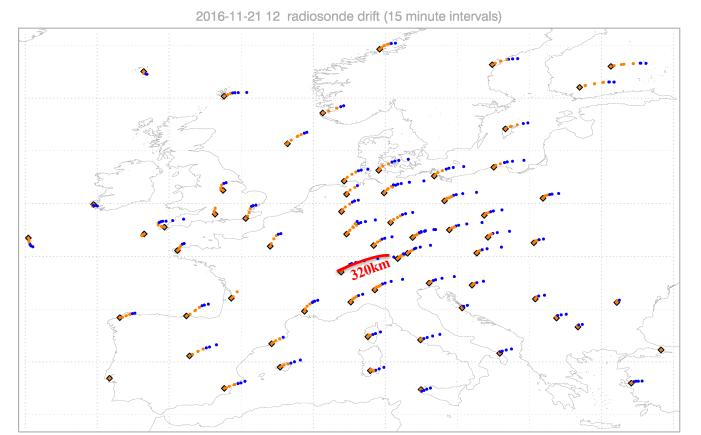
Bruce Ingleby, ECMWF

Accounting for radiosonde drift in data assimilation (we are improving the forward model *H* and reducing forward model error statistics, F)

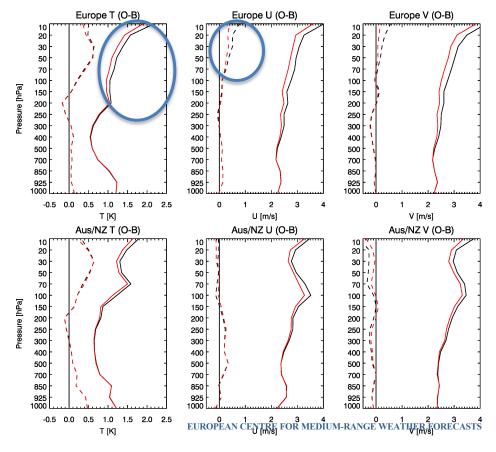
- "Old style" radiosondes only provide the balloon launch location
- Native BUFR reports provides accurate location/time for each measurement
- The location/time information can be used to account for balloon drift in data assimilation
- We split the ascent into 15 minute chunks
- Was implemented at ECMWF in June 2018
- BUFR DROP (high-resolution dropsonde data was implemented at ECMWF in June 2019)
- In addition, descent data from BUFR radiosondes in Germany is now being used.

Example of large drift of radiosonde on a windy day

- Black diamonds launch, levels to 100 hPa, levels above 100 hPa
- BUFR data not available for all countries at the time of this figure (Nov 2016)



Impact of accounting for radiosonde drift in data assimilation Mean and rms o-b statistics: Nov 2016



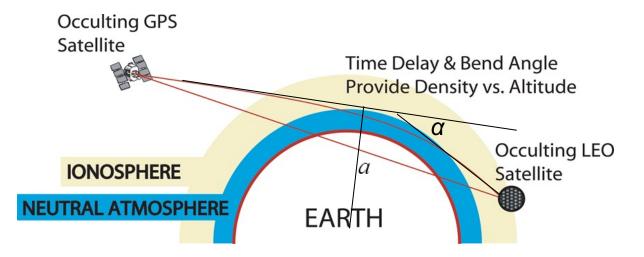
• Assimilated BUFR TEMP standard levels only (to get clean comparison)

 Good improvements at 200 hPa and above – including wind biases

Active satellite observation types

- More complicated forward operators, *H*. Global datasets
 - GNSS Radio Occultation
 - Scatterometer
 - Altimeter
 - Aeolus

Global Navigation Satellite System Radio Occultations GNSS RO (GPS RO) geometry



As the LEO moves behind the Earth we obtain a profile of bending angles. The forward model $H(\mathbf{x})$ computes bending angle as a function of impact parameter (height), $\alpha(a)$.

The bending angle depends on temperature, humidity and pressure.

Global Navigation Satellite System Radio Occultations GNSS RO (GPS RO) geometry



Key characteristics

Time Delay & Bend Angle Provide Density vs. Altitude

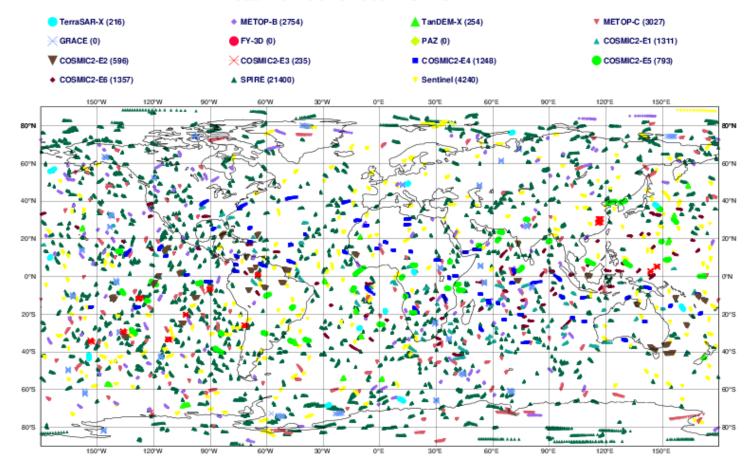
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 Limb geometry mean very good vertical resolution

Can be assimilated without bias correction

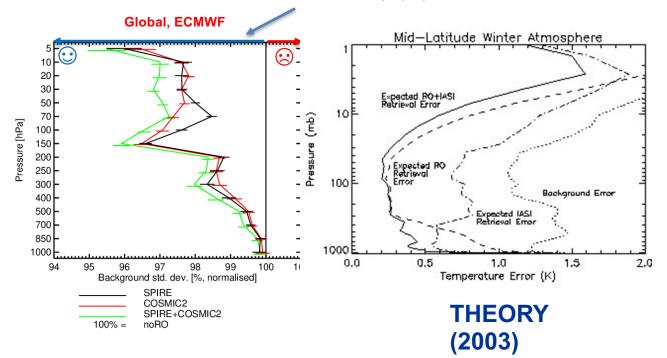
The bending angle depends on temperature, humidity and pressure.

ECMWF data coverage (used observations) - GPSRO 2023052103 to 2023052109 Total number of obs = 37431



GNSS-RO has biggest impact in upper-troposphere/stratosphere Fits to **radiosonde temperature** observations

Normalised standard deviation in (o-b) departure



Scatterometer

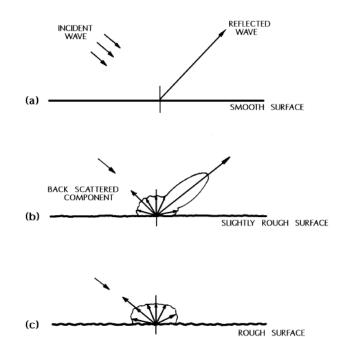
- ✓ A Scatterometer is an active microwave instrument (side-looking radar)
 - Day and night acquisition
 - Not affected by clouds
- ✓ The return signal, *backscatter* (σ_0 *sigma-nought*), is sensitive to:
 - Surface wind (ocean)
 - Soil moisture (land)
 - Ice age (ice)



- ✓ Scatterometer was originally designed to measure ocean wind vectors:
 - Measurements sensitive to the ocean-surface roughness due to capillary gravity waves generated by local wind conditions (surface stress)
 - Observations from different look angles: wind direction



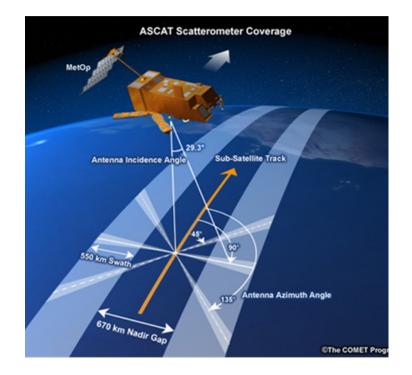
Dependency of the backscatter on... Wind speed











EG, ASCAT

We measure be back scatter from three directions

• Fore/mid/aft

Triplet of backscatters used in a geophysical model function (GMF) to provide vector wind information.

But the vector wind solutions are ambiguous!

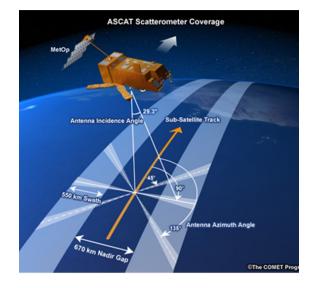
How can we relate backscatter to wind speed and direction?

The relationship is determined empirically by developing a Geophysical Model Function (**GMF**)

- Ideally collocate with surface stress observations
- In practice with buoy and 10m model winds

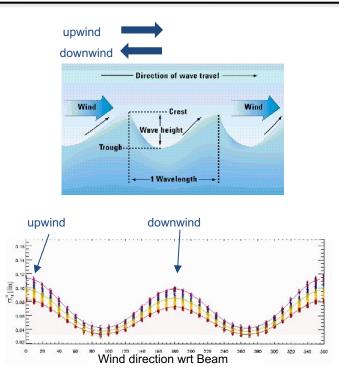
 $\sigma_0 = GMF(U_{10N}, \phi, \theta, p, \lambda)$

- U_{10N}: equivalent neutral wind speed
- ϕ : wind direction w.r.t. beam pointing
- θ : incidence angle
- *p* : radar beam polarization
- λ : microwave wavelength



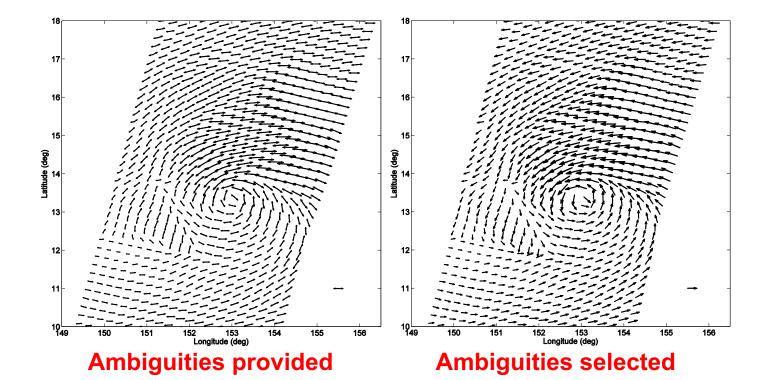
Dependency of the backscatter on... Wind direction





Wind Direction Ambiguity removal

- Each wind vector cell has usually two possible solutions for wind direction and speed
- The correct solution is determined during the 4D-Var

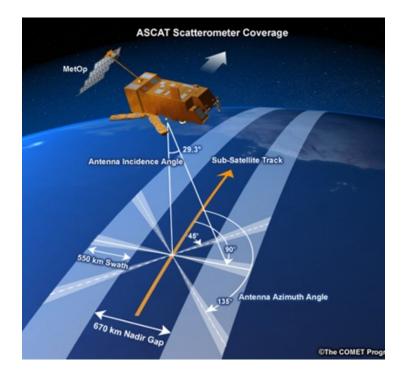


Past, present and future scatterometers

Used on European platforms (1991 onwards):
✓ SCAT on ERS-1, ERS-2 by ESA
✓ ASCAT on Metop-B/C by EUMETSAT
✓ SCAT on EPS-SG planned until 2040

- Frequency ~5.3 GHz
- Wavelength ~5.7 cm
- Three antennae
 - Enables estimation of both wind speed and wind direction

Also Chinese scatterometer data available now:



✓ HY-2B
✓ HY-2C and HY-2D being tested
✓ Windrad

Why is Scatterometer important?

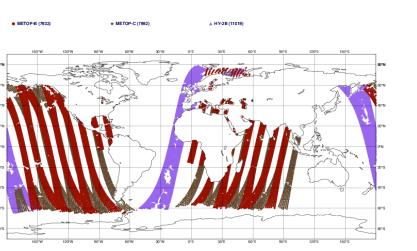
The scatterometer provides the ocean surface wind information (ocean wind vectors).

Ocean surface winds:

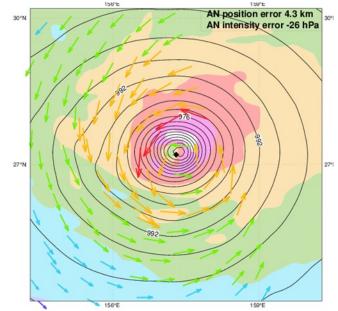
- affect the full range of ocean movement
- modulate air-sea exchanges of heat, momentum, gases, and particulates
- direct impact on human activities

ECMWF data coverage (used observations) - SCATTEROMETER

2023052103 to 2023052109Total number of obs = 26943



Important data source in tropical cyclones (We thin more than this)



Some ideas being pursued in SCAT usage

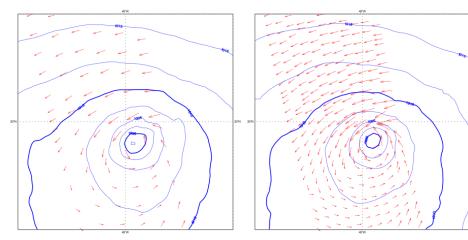
· Increasing the usage (reducing the thinning applied)

• SCAT observation sensitive to the relative motion between the atmosphere and ocean

- At the moment, we ignore the ocean current but we can add this information to forward model
- Is SCAT impact limited currently by model error/bias?
 - We will test a bias corrected dataset to investigate this

- Test the direct assimilation of sigma0 rather than assimilating ambiguous vector winds
 - we now handle non-linearity better in DA

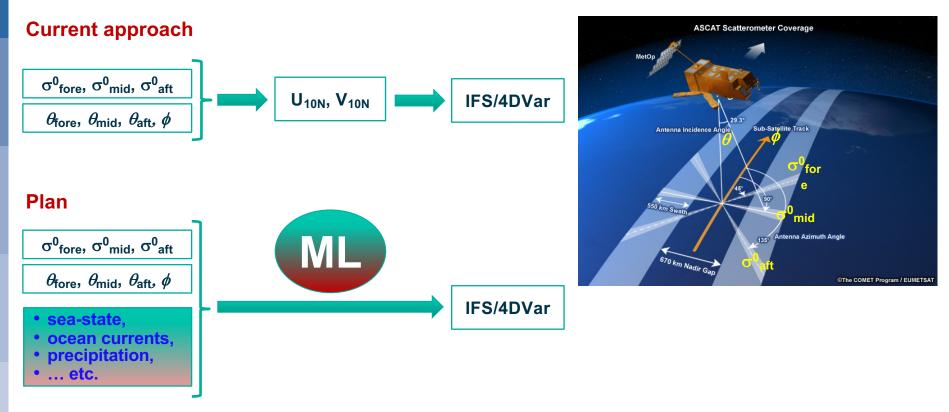
- **Revisit** the SCAT sigma0 problem and train a neural network to compute $\sigma_0 = GMF(U_{10N}, \phi, \theta, p, \lambda)$



100 km thin

50 km (48R1)

SCATT Data Assimilation

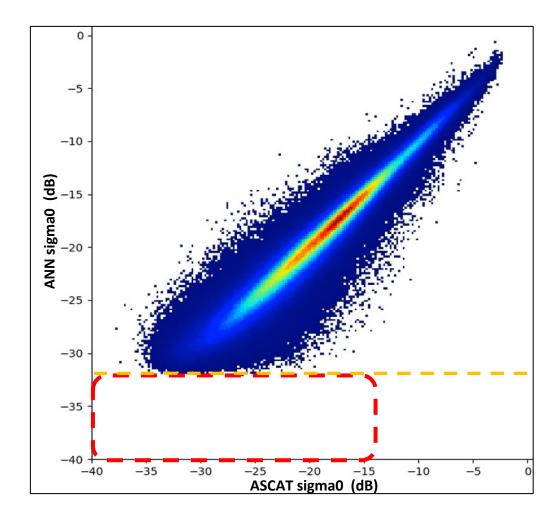


Training against model first guess (FG) wind

- N = 1266843
- Bias = 0.0133 dB
- SDD = 1.3089 dB
- R = 0.96848

CECMWF

 ANN is not able to extract any information from sigma0 below ~ -31.5 dB!

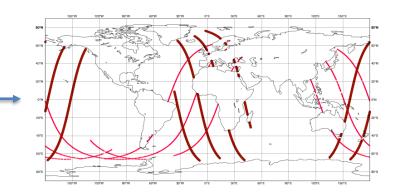


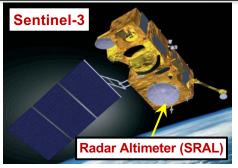
Radar Altimeters

- ✓ Radar altimeter is a nadir looking instrument.
- ✓ Specular reflection.
- Electromagnetic wave bands used in altimeters:
 - Primary:
 - Ku-band (~ 2.5 cm) ERS-1/2, Envisat, Jason-1/2/3, Sentinel-3A/B
 - Ka-band (~ 0.8 cm) SARAL/AltiKa (only example)
 - Secondary:
 - C-band (~ 5.5 cm) Jason-1/2/3, Topex, Sentinel-3,
 - S-band (~ 9.0 cm) Envisat
- Main parameters *retrieved* from an altimeter:
 - Sea surface height (ocean model)
 - Significant wave height (wave model)
 - Wind speed retrievals (used for verification)

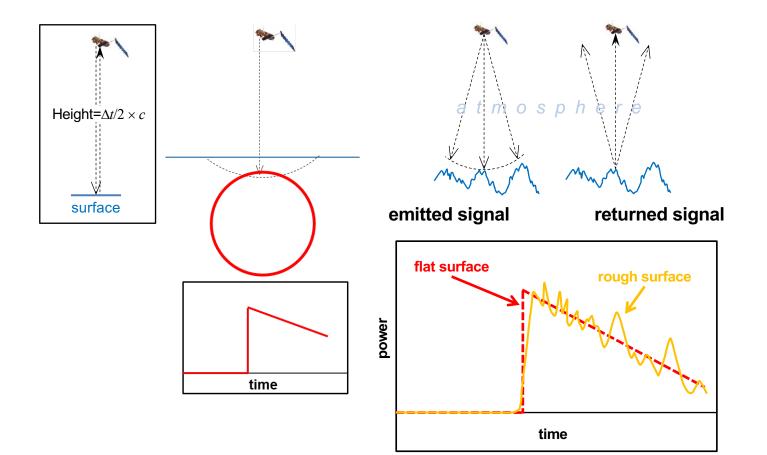
ECMWF data coverage (used observations) - WAVE HEIGHT 2023052103 to 2023052109 Total number of obs = 1966

JASON-3 (1013

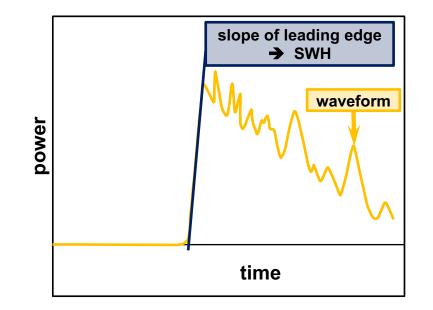




How Altimeter Works

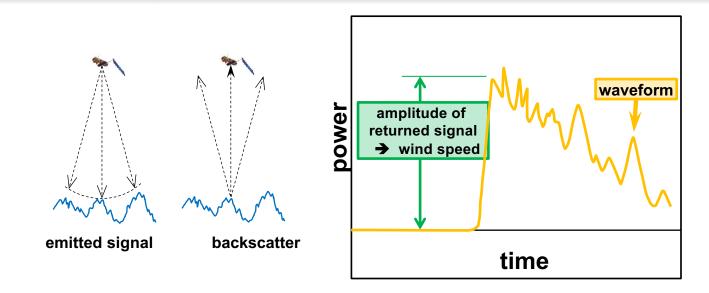


Significant Wave Height (SWH)



- ✓ SWH is the mean height of highest 1/3 of the surface ocean waves
- ✓ Higher SWH \rightarrow smaller slope of waveform leading edge
- Errors are mainly due to waveform retracking (algorithm) and instrument characterisation.

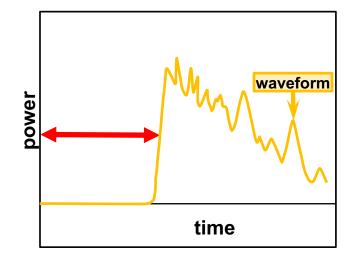
Surface wind speed



Backscatter is related to water surface Mean Square Slope (MSS)

- ✓ MSS can be related to wind speed
- ✓ Stronger wind → higher MSS → smaller backscatter
- Errors are mainly due to algorithm assumptions, waveform retracking (algorithm), unaccounted-for attenuation & backscatter.

Sea Surface Height

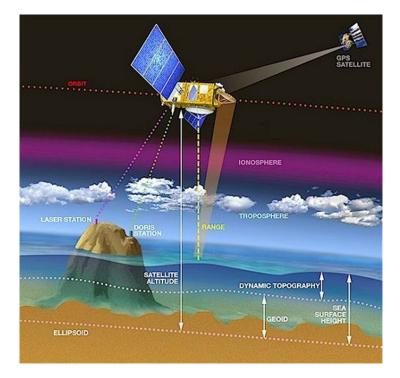


 \checkmark Time delay \rightarrow sea surface height

- Radar signal attenuation due to the atmosphere is caused by:
 - Water vapour impact: ~ 10's cm.
 - Dry air impact: ~ 2.0 m

Correction made using radiometer and model data

Altimeter *corrections* applied to sea surface height



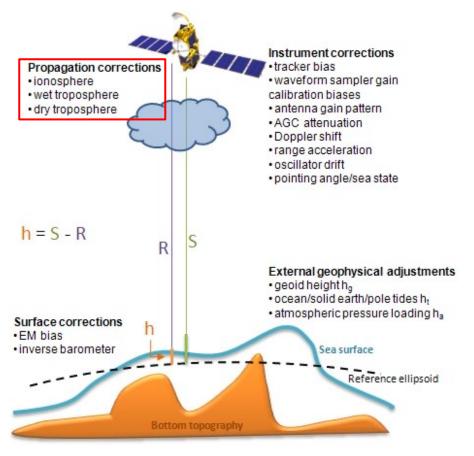
Sea Surface Height = Satellite altitude – Range - Corrections



Corrections to sea surface height measurements

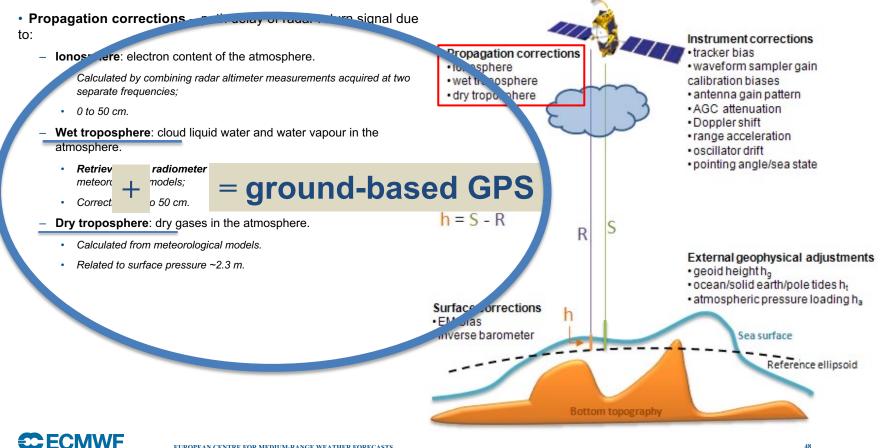
 Propagation corrections – path delay of radar return signal due to:

- **lonosphere**: electron content of the atmosphere.
 - Calculated by combining radar altimeter measurements acquired at two separate frequencies;
 - 0 to 50 cm.
- Wet troposphere: cloud liquid water and water vapour in the atmosphere.
 - Retrieved from radiometer measurements and/or estimated from meteorological models;
 - Correction ~ 0 to 50 cm.
- Dry troposphere: dry gases in the atmosphere.
 - Calculated from meteorological models.
 - Related to surface pressure ~2.3 m.





Corrections to sea surface height measurements



Aeolus – technology demonstration

 Earth observation satellite. 5th satellite launched (22 Aug 2018) in ESA's Earth Explorer programme – a technology demonstration

• **Scientific payload:** UV Doppler wind lidar measuring profiles of line-of-sight wind information (06/18 hour local solar time)

- Also provides profiles of aerosol and cloud backscatter and extinction

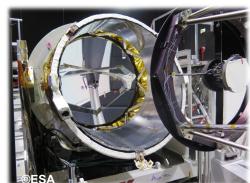
- Main goal is to improve weather forecasts by *partially filling the gap in wind profiles (as stated by WMO RRR 2018)* and improve understanding of the atmospheric dynamics
- Operationally assimilated at ECMWF since 9 January 2020 also at DWD, Météo-France since summer 2020, and the Met Office Dec 2020.

- Ended May 1, 2023
- Aeolus-2 expected around 2032





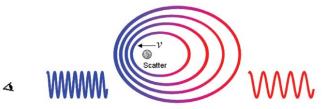




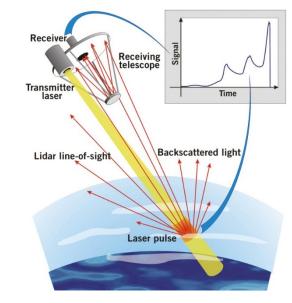
Doppler wind lidar

• Measure Doppler frequency shift of backscattered laser light

2



- Doppler shift, $\Delta f = 2f_0 v_{LOS}/c$
 - Simple in principle
 - But frequency shift is *tiny*: $\frac{\Delta f}{f_0} \sim 10^{-8}$
 - 1 m/s change ~ 5.6 MHz (2.4 fm)
- For Aeolus (UV), scattering from:
 - Rayleigh scattering from air molecules
 - Mie scattering from particles (aerosol/cloud)
 - Wind = Average speed of movement of scatterers in volume of air





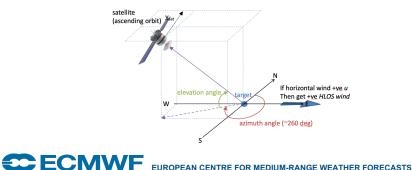
Forward model

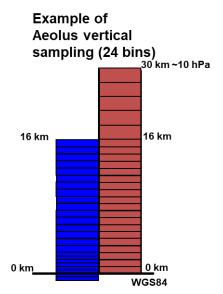
- Compute point line of sight wind value near centre of vertical bins
- Forward model computes

$$H(\mathbf{x}) = -u\sin\phi - v\cos\phi$$

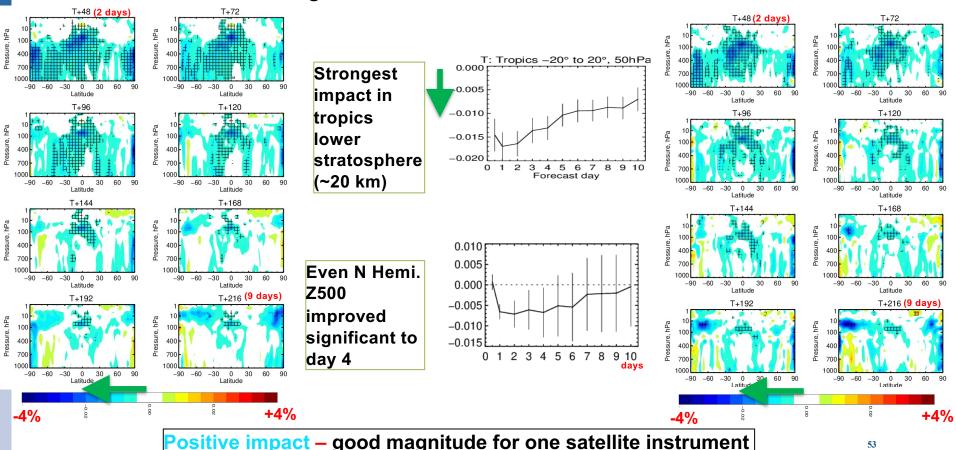
at the observation height using the forecast (u, v)

 \emptyset is the azimuth angle, describing the line-of-sight pointing of the laser projected onto the horizontal plane





Aeolus significantly improves NWP forecasts in most areas and forecast ranges

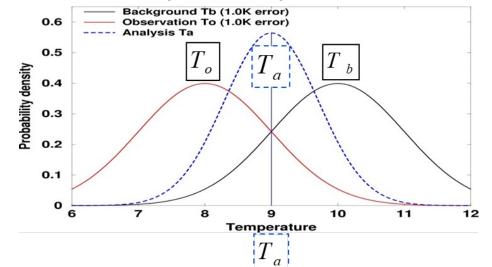


Vector wind RMSE zonal average

Temperature RMSE zonal average

Quality Control (QC) Really important – but getting squeezed as training course grows

QC: The linear scalar temperature problem

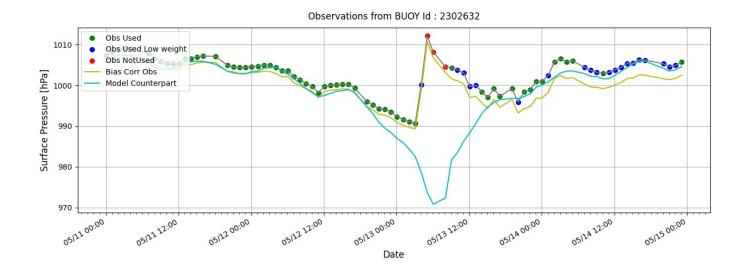


- Both the **standard deviation** of the background and observation errors and the observation errors are 1 K. The **assumed error statistics** determine the "gain matrix", K.
- If these errors are uncorrelated, the st. dev. of $(T_o T_b)$ differences should be **about** $\sqrt{2}$ K.
- All observations have errors we accept that (**R** matrix). But what should we make of a difference of, say, $(T_o T_b) > 20$ K? The **actual errors** in this case are probably not consistent with the error statistics we've assumed in the K matrix.

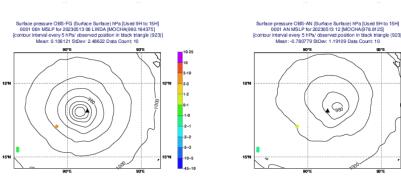
Large departures can be caused by ...

• Either the observation errors are large or the background (forecast) errors are large

• A real example that caused problems at ECMWF last week: TC Mocha May 13

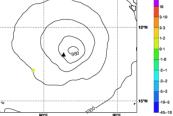


TC Mocha

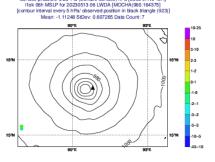


Operations





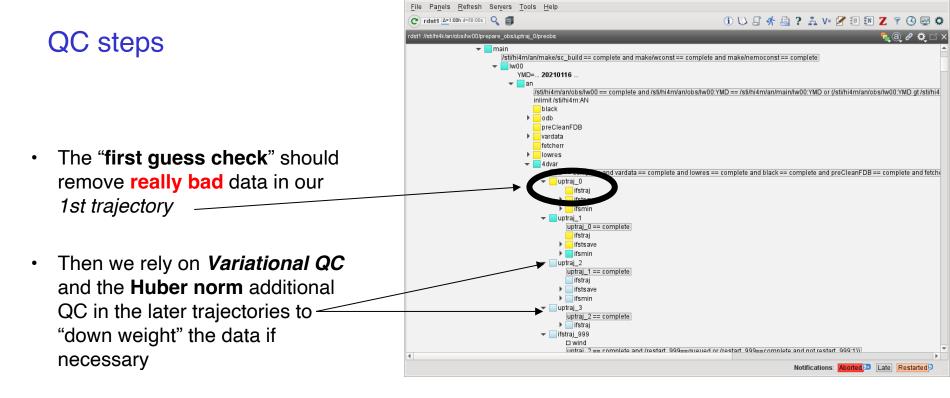
Remove ob



Surface pressure OBS-FG (Surface Surface) hPa [Used 9H to 15H]



Surface pressure OBS-AN (Surface Surface) hPa [Used 9H to 15H] i1ek AN MSLP for 20230513 12 [MOCHA(957.770625] [contour interval every 5 hPa/ observed position in black triangle (923)] Mean: -0.402938 StDev: 0.269854 Data Count: 7



 Current testing at ECMWF Also include Variational QC/Huber in 1st trajectory? Q. J. R. Meteorol. Soc. (1999), 125, pp. 697-722

Variational quality control

By ERIK ANDERSSON* and HEIKKI JÄRVINEN European Centre for Medium-Range Weather Forecasts, UK

What is the probability of an (o-b) of this size given R and B? Normal departures and gross errors have different distributions

$$p^{\rm QC} = (1 - A)N + Ap^{\rm G}$$

The a priori probability of gross error

Assumed distributions

• The gross errors have a flat distribution

$$p^{G} = \frac{1}{2d}$$

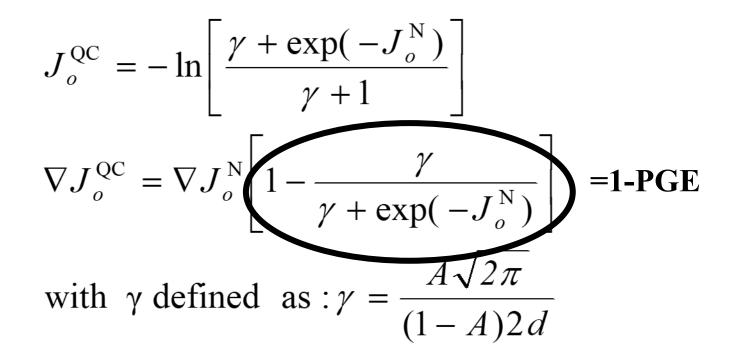
• The ordinary departures a normally distribruted

$$N = \frac{1}{\sigma_o \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{y - Hx}{\sigma_o}\right)^2\right]$$

Take
$$-\ln(P^{QC})=J_0^{QC}$$

$$J_o^{\text{QC}} = -\ln\left[\frac{\gamma + \exp(-J_o^{\text{N}})}{\gamma + 1}\right]$$
$$\nabla J_o^{\text{QC}} = \nabla J_o^{\text{N}} \left[1 - \frac{\gamma}{\gamma + \exp(-J_o^{\text{N}})}\right]$$
with γ defined as $: \gamma = \frac{A\sqrt{2\pi}}{(1 - A)2d}$

Take
$$-\ln(P^{QC})=J_0^{QC}$$



So we <u>weight</u> the (o-b) departures by 1 minus the Probability of Gross Error (PGE). The <u>a priori</u> PGE, A, is updated based on the size of the (o-b) departure using *Bayes Theorem*!

The large (o-b) of 20 K in our scalar example would be multiplied by (1-PGE)

$$\nabla J_o^{\text{QC}} = \nabla J_o^{\text{N}} \left(1 - \frac{\gamma}{\gamma + \exp(-J_o^{\text{N}})} \right) = 1 - PGE$$

with γ defined as $: \gamma = \frac{A\sqrt{2\pi}}{(1 - A)2d}$

In recent years we have also used the Huber norm

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On the use of a Huber norm for observation quality control in the ECMWF 4D-Var

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*Correspondence to: L. Isaksen, ECMWF, Shinfield Park, Reading RG2 9AX, UK. E-mail: lars.isaksen@ecmwf.int The Huber norm is less conservative than VarQC

$$f(x) = \frac{1}{\sigma_o \sqrt{2\pi}} \exp\left\{-\frac{\rho(x)}{2}\right\}$$
(1)

with

$$\rho(x) = \begin{cases} \frac{x^2}{\sigma_o^2} \\ \frac{2c|x| - c^2}{\sigma_o^2} \end{cases}$$

for
$$|x| \le c$$
,
(2)
for $|x| > c$,
 $x = y - H(\mathbf{x})$, the (o-b) in
our terminology/notation!

The Huber norm is less conservative than VarQC

with

$$f(x) = \frac{1}{\sigma_o \sqrt{2\pi}} \exp\left\{-\frac{\rho(x)}{2}\right\}$$
Derived from
departure
statistics
Can be
asymmetric
either side of
peak.

$$x = y - H(\mathbf{x}), \text{ the (o-b) in}$$

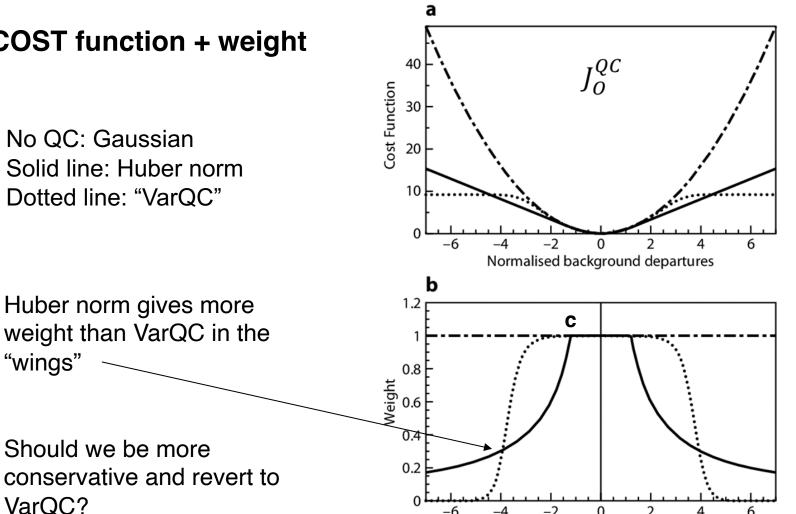
our terminology/notation!

COST function + weight

No QC: Gaussian Solid line: Huber norm Dotted line: "VarQC"

"wings"

VarQC?



Normalised background departures

Summary

- Reviewed basics of data assimilation
 - Gain matrix, K
 - Use of error statistics to provide the weighting, R
 - observation operator, $H(\mathbf{x})$
- Impact of in situ and actively sensed observations in global NWP
 - Impact of the data types, how we assimilate the data
- Quality control: introduced the VarQC and Huber norm approach used at ECMWF
 - We need to screen out cases when their errors are not consistent with R
 - More work to do in this area/ongoing debate at ECMWF