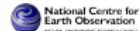


Introduction to Data Assimilation

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Outline

- 1 What is data assimilation (DA)?
- 2 From Bayes' Rule to DA
 - Assessing the update
- 3 DA methods
 - Variational schemes
 - Sequential methods: Filters & Smoothers
 - MCMC
- 4 Some DA examples
 - CCDAS
 - EnKF & DALEC model
 - JRC-TIP
 - EO-LDAS
- 5 Discussion

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We have seen *models* and *observations*

Models Can be wrong (missing processes, inadequate parametrisation, uncertainty in drivers, . . .)

Observation Have uncertainty, may be missing or might not reflect the quantity of interest directly.

DA provides an statistical framework that optimally combines *observations* and *models*, plus all the associated *uncertainties* to **infer** the most likely state of the land surface, plus uncertainties.

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Observation operators

- Typically, the state vector \vec{x} (LAI, soil moisture...) is **not directly observable**.
- Need to *map* from \vec{x} to the observations (e.g. backscatter, reflectance, temperature brightness) using an **Observation Operator** $\mathcal{H}(\vec{x})$.
- Observations \vec{y} are corrupted by **additive Gaussian noise** ϵ_{obs} .

The measurement equation is then simply:

$$\mathcal{H}(\vec{x}, l) = \vec{y} + \epsilon_{obs} \quad (1)$$

We want to estimate the \vec{x} based on the data. How do we go about that?

Least Squares

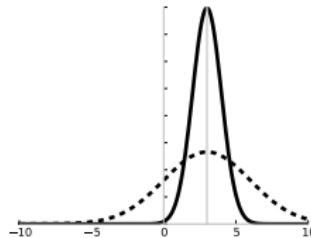
A way to find the solution to the measurement equation is to find a set of parameters \vec{x}_0 that **minimise** the difference between predicted observation and actual observation, modulated by the uncertainty in the observations:

$$\|\mathcal{H}(\vec{x}, I) - \vec{y}\|^2 \leq \epsilon_{obs} \quad (2)$$

This means that there are **infinite solutions** that meet the criterion in Eq. 2! The problem is said to be *ill posed*. The only practical way to solve this underdetermination is by adding extra constraints.

Probability

We can't avoid ill posedness. One way around it is to assume we no longer have discrete parameters, but **parameter distributions**. The distribution encompasses our current belief in the value of the parameter.



Our problem is now how to express $p(\vec{x}|\vec{y})$, the probability of the state \vec{x} **conditioned on** the observations, \vec{y} .

Bayes' Rule

$$\underbrace{p(\vec{x}|y)}_{\text{Posterior}} = \frac{\underbrace{p(y|\vec{x})}_{\text{Likelihood}} \cdot \underbrace{p(\vec{x})}_{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}, \quad (3)$$

The **likelihood** is derived from the mismatch of the model to the observations using an observation operator

The **prior** is a pdf of any knowledge we might have about the state before the observations are considered

Simple univariate example

Try to infer x from y , using an identity observation operator (i.e., $x = y$) and Gaussian noise:

$$p(y|x) = \frac{1}{\sqrt{2\pi}\sigma_{obs}} \exp\left[-\frac{1}{2}\frac{(x-y)^2}{\sigma_{obs}^2}\right]. \quad \text{Likelihood} \quad (4)$$

Assume that we only know that x is Gaussian distributed with μ_p and σ_0 :

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma_0} \exp\left[-\frac{1}{2}\frac{(x-\mu_p)^2}{\sigma_0^2}\right] \quad \text{Prior} \quad (5)$$

$$p(x|y) \propto \frac{1}{\sigma_{obs}\sigma_0} \exp\left[-\frac{1}{2}\frac{(x-\mu_p)^2}{\sigma_0^2}\right] \cdot \exp\left[-\frac{1}{2}\frac{(x-y)^2}{\sigma_{obs}^2}\right]. \quad \text{Posterior} \quad (6)$$

Simple univariate example(II)

The posterior distribution is indeed a Gaussian, and its mean and std dev can be expressed as an **update** on the prior values:

$$\mu_p = \mu_0 + \frac{\sigma_0^2}{\sigma_0^2 + \sigma_{obs}^2} (y - \mu_0). \quad (7)$$

$$\sigma_p^2 = \sigma_0^2 \cdot \left(1 - \frac{\sigma_0^2}{\sigma_0^2 + \sigma_{obs}^2}\right), \quad (8)$$

Univariate example (III)

$$p(x) \sim \mathcal{N}(\mu = -5, \sigma^2 = 1) \quad p(y|x) \sim \mathcal{N}(0, 4) \quad p(x|y) \sim \mathcal{N}(-4, 2/5)$$

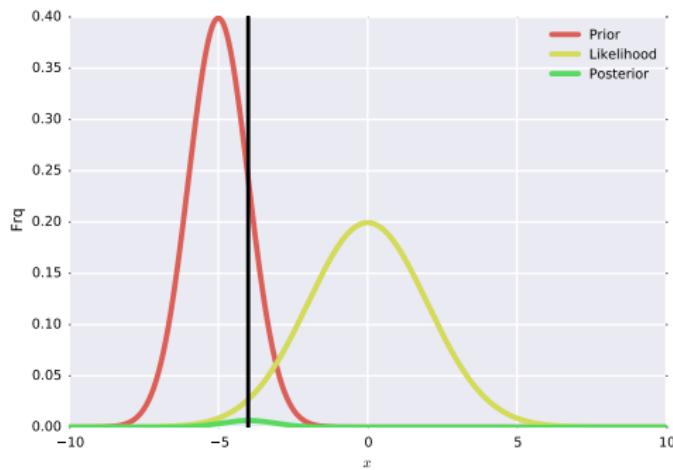


Figure: The prior (red), the likelihood (yellow) and the posterior (green) for the simple 1D case. The black lines indicates the maximum *a posteriori*.

Multivariate example (I)

\vec{x} (the state) is a **vector**, rather than a scalar as above. The Gaussian pdf for \vec{x} is given by

$$P_b(\vec{x}) = \frac{1}{(2\pi)^{\frac{n}{2}} \sqrt{\det(\mathbf{B})}} \exp \left[-\frac{1}{2} (\vec{x}_b - \vec{x})^\top \mathbf{B}^{-1} (\vec{x}_b - \vec{x}) \right], \quad (9)$$

where n is the size of \vec{x} , \vec{x}_b is the mean vector, \mathbf{B} is the covariance matrix and $^\top$ indicates transposition. \mathbf{B} indicates the covariance between the elements of \vec{x} . For a two dimensional case, we have

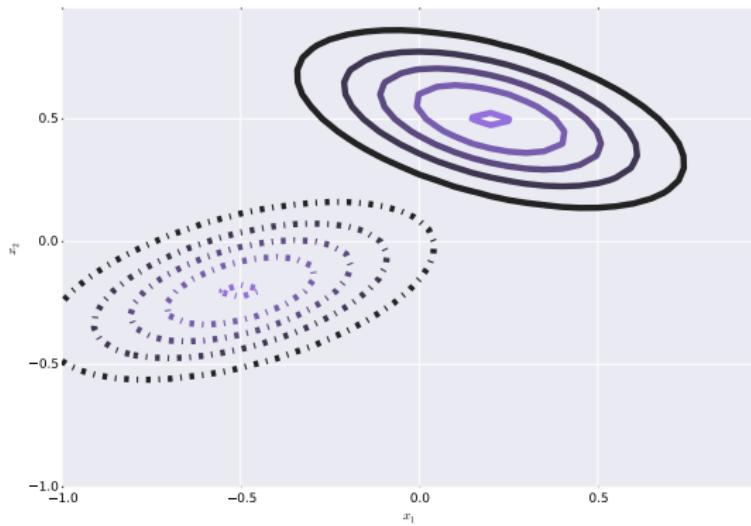
$$\mathbf{B} = \begin{bmatrix} \sigma_0^2 & \rho_{0,1}\sigma_0\sigma_1 \\ \rho_{0,1}\sigma_0\sigma_1 & \sigma_1^2 \end{bmatrix} \quad (10)$$

Again, posterior is Gaussian if prior and likelihood are Gaussian and observation operator linear

Multivariate example (II)

$\vec{x} = [0.2, 0.5]^\top$ $\vec{x} = [-0.5, -0.2]^\top$. Covariance is

$$\mathbf{B} = \begin{bmatrix} 0.3^2 & \pm 0.5 \times 0.3 \times 0.2 \\ \pm 0.5 \times 0.3 \times 0.2 & 0.2^2 \end{bmatrix}, \quad (11)$$



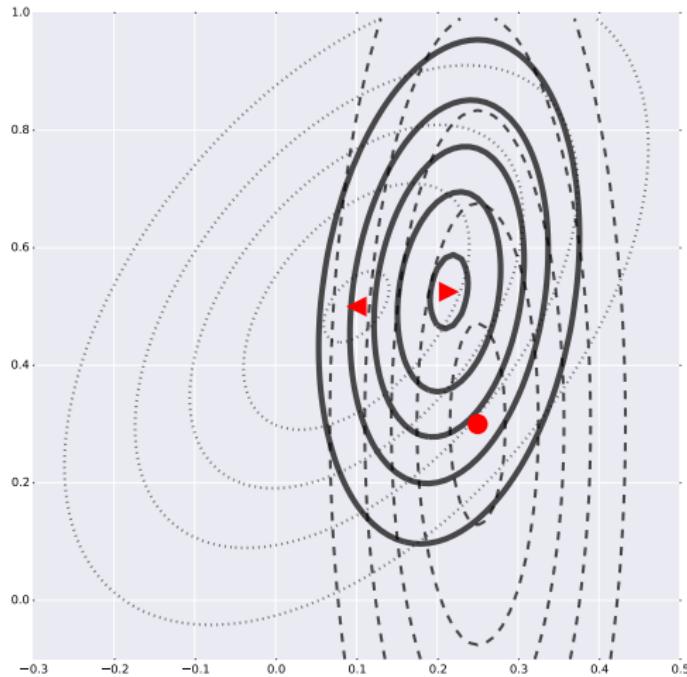
Multivariate example (III)

Since the posterior is Gaussian, we can write update equations:

$$\begin{aligned}\vec{x}' &= \vec{x}_b + \mathbf{B} \mathbf{H}^\top \left(\mathbf{H} \mathbf{B} \mathbf{H}^\top + \mathbf{R} \right)^{-1} (\vec{y} - \mathbf{H} \vec{x}) \\ &= \vec{x}_b + \mathbf{K} \cdot (\vec{y} - \mathbf{H} \vec{x}).\end{aligned}\tag{12}$$

$$\mathbf{Q} = (\mathbf{I} - \mathbf{K} \mathbf{H}) \mathbf{B}.\tag{13}$$

Multivariate example (IV)



Multivariate example (V)

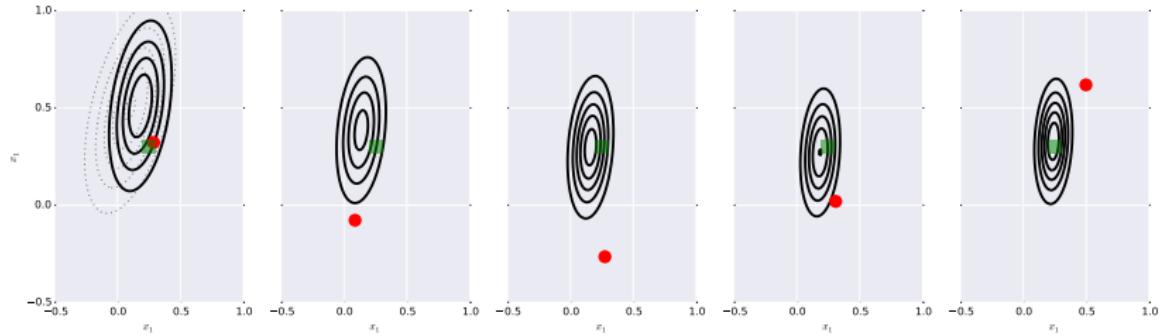


Figure: The prior (dotted line, only shown in the first panel), and the posterior (full line) for the sequential experiment. Each panel, from left to right, represents the ingestion of a new observation, drawn from a distribution centred in the location of the green square, and whose value is indicated by the red circle.

Assessing the effectiveness of the update

Use **relative entropy**: the difference between prior and posterior! Relative entropy can be expressed as *dispersion* of the posterior \mathbf{C}_{post} relative to the prior \mathbf{C}_{prior} :

$$D = \frac{1}{2} \left[\ln \left(\frac{\det \mathbf{C}_b}{\det \mathbf{C}_{post}} \right) + \text{tr}(\mathbf{C}_{post} \mathbf{C}_b^{-1}) - n \right], \quad (14)$$

where $\text{tr}(\mathbf{C})$ denotes the *trace* operator (the sum of the diagonal elements) and n is the rank of the matrix (the number of elements in \vec{x}). Another metric is a form of 'distance' moved by the mean state relative to the prior uncertainty in going from the prior mean to the posterior (the 'signal'):

$$S = \frac{1}{2} (\vec{x}_{post} - \vec{x}_b)^\top \mathbf{C}_b^{-1} (\vec{x}_{post} - \vec{x}_b) \quad (15)$$

$$E = \frac{D + S}{\ln 2},$$

Some comments on priors

A prior is **everything** that is known about a magnitude. This information includes:

- Parameter boundaries
- Expectations of smoothness
- Temporal (or spatial) trajectories for parameters, derived from a DGVM
- Experts choice
- Etc.

Summary

- DA is basically Bayes' Rule
- The likelihood is how we incorporate observations, using an Observation Operator to map from state to observation space
- The prior is typically just an expectation on the value of the parameter, but can be many other things
- If things are

- 1 Gaussian
- 2 Linear

... Then the posterior is Gaussian too

- We can see DA as an update of the prior when new evidence is included

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Variational schemes (4DVAR and 3DVAR)

Variational schemes start by writing the $-\log$ posterior, and minimise it to find the most likely value of \vec{x}

$$J(\vec{x}) = \log p(\vec{x}|\vec{y}) = \underbrace{[\vec{x} - \vec{x}_b]^\top \mathbf{C}_b^{-1} [\vec{x} - \vec{x}_b]}_{\text{Fit to Prior}} + \underbrace{[\vec{y} - \mathcal{H}(\vec{x})]^\top \mathbf{C}_{obs}^{-1} [\vec{y} - \mathcal{H}(\vec{x})]}_{\text{Fit to Observations}} \quad (17)$$

\vec{x}_b Prior mean vector

\vec{y} Observations vector

$\mathcal{H}(\vec{x})$ Observation operator acting on state

\mathbf{C}_b Prior covariance matrix

\mathbf{C}_{obs} Obs covariance matrix

“Strong” constraint

$$J_{obs}(\vec{x}) = [\vec{y} - \mathcal{H}(\vec{x})]^\top \mathbf{C}_{obs}^{-1} [\vec{y} - \mathcal{H}(\vec{x})] \quad (18)$$

We assume that the mapping is from \vec{x} to \vec{y} using ObsOp \mathcal{H} . However, we assume that this mapping is **perfect**: for a particular state value, the ObsOp will produce the required observation, without the additive noise.

Strong constraint The solution **must** be in the space of \mathcal{H} . E.g. if solving for parameters in a DGVM, and then mapping from LAI to reflectance using an RT scheme, the solution will be compatible with the DGVM and RT scheme. This can be a major problem as models are often **very wrong!**

Weak constraint The solution needs not be in the domain of the model.
This assumes **model error**

“Weak” constraint

$$\begin{aligned} J(\vec{x}) = & (\vec{x} - \vec{x}_b)^\top \mathbf{C}_b^{-1} (\vec{x} - \vec{x}_b) \\ & + (\vec{y} - \mathcal{H}(\vec{x}))^\top \mathbf{C}_{obs}^{-1} (\vec{y} - \mathcal{H}(\vec{x})) \\ & + (\vec{x} - \mathcal{M}(\vec{x}))^\top \mathbf{C}_{model}^{-1} (\vec{x} - \mathcal{M}(\vec{x})) \end{aligned} \quad (19)$$

In a weak constraint system, the solution \vec{x}_s might not be a value that can be produced by \mathcal{M} , but \mathbf{C}_{model} will indicate how much the solution can deviate from the model. Estimating the model error is typically quite hard.

Smoothness priors

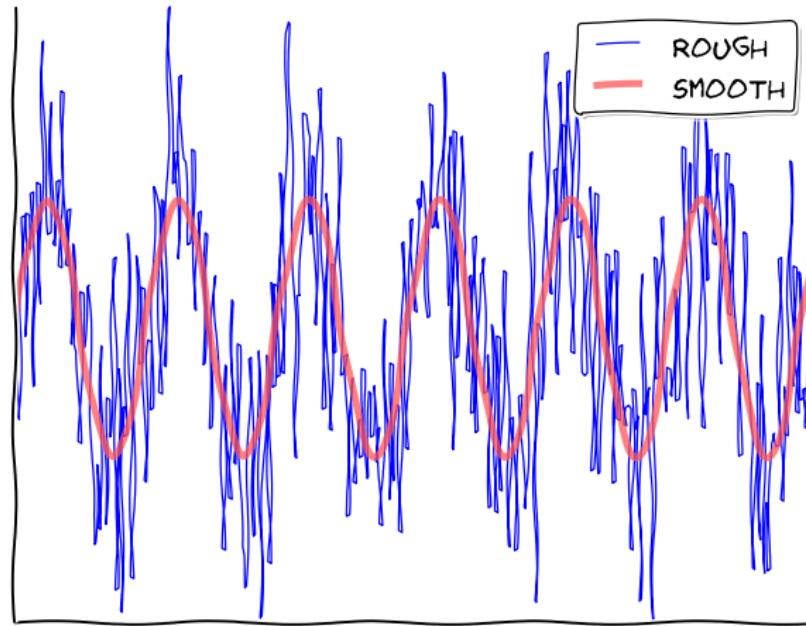
- Spatial/temporal evolution of many geophysical fields is **smooth**. How can we integrate this knowledge into DA?
- We can think of an extra constraint that “penalises” rough trajectories
- Smooth trajectories characterised by 1st order differences ~ 0 , rough trajectories 1st order difference are large
- So model $\mathcal{M}(\vec{x}) \rightsquigarrow \vec{x}_{k+1} = \vec{x}_k + \epsilon_{mod}$

$$J_{smooth} = \frac{1}{2} (\Delta \vec{x})^\top \mathbf{C}_{\text{smooth}}^{-1} (\Delta \vec{x}) \quad (20)$$

$$\Delta = \begin{bmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ \vdots & \ddots & \ddots & \dots & -1 & 0 \\ 0 & 0 & 0 & \dots & 1 & -1 \end{bmatrix} \quad (21)$$

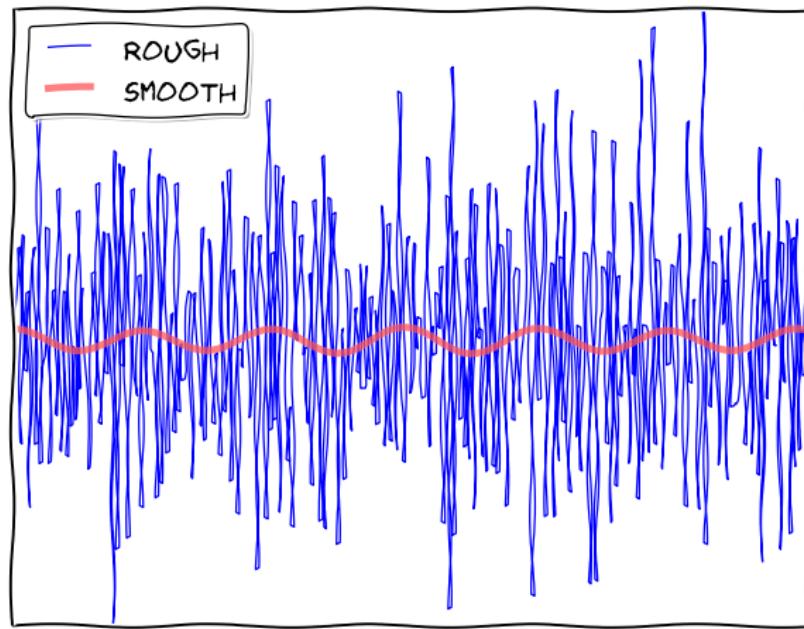
Smoothness priors

For this example, the mean sum of squared first order differences is 0.07 for the smooth time series, and 1.06 for the rough!



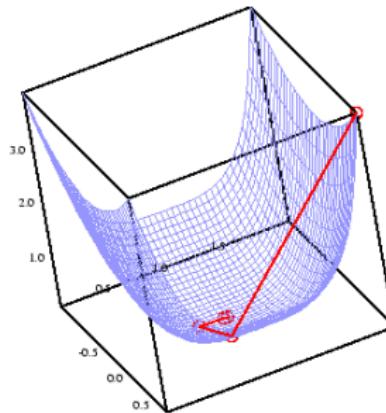
Smoothness priors

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Solving the variational problem

Typically, we use **gradient descent** methods that require the partial derivatives of the cost function.



Uncertainty is calculated by looking at the **matrix of second partial derivatives**, the **Hessian**

- ~ For linear ObsOp& Gaussian, the Hessian is the inverse of the posterior covariance matrix!

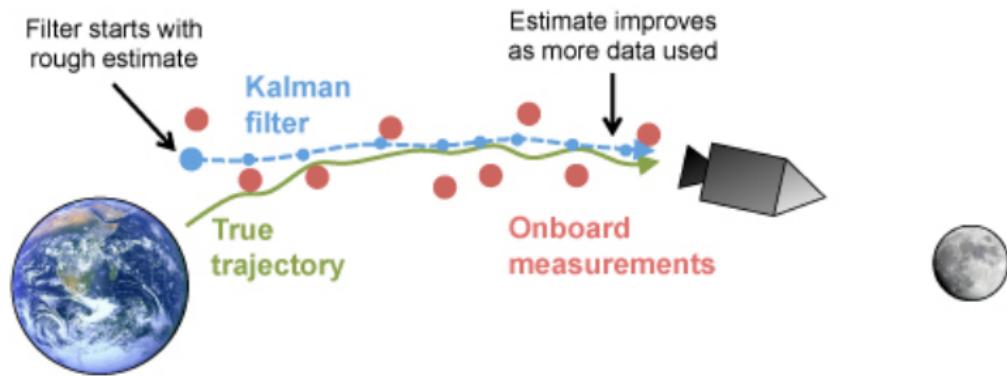
Summary

Variational methods (inc 3dVAR and 4dVAR) **minimise a cost function**, derived from the logarithm of the posterior

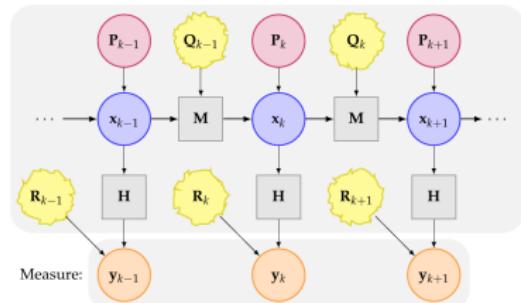
- Weak & strong constraint flavours to deal with model error
- Very flexible: if sources of information are **independent**, you just add more terms to the cost function
- Minimisation is computationally expensive (particularly if the state vector is large).
- Exploit having partial derivatives to use gradient descent methods
- The posterior covariance matrix is approximated by the inverse of the Hessian at the minimum
- Look out for local minima!

Sequential methods

- Use the updating concept: the posterior of time $k - 1$ is the prior of time k .
- The state and its associated uncertainty \mathbf{P}_{k-1} are propagated using a **trajectory model** $\mathbf{M} \rightsquigarrow \vec{x}_k = \mathbf{M}\vec{x}_{k-1}$
- Kalman filter is a good example, heritage from position tracking



The Kalman filter



Assumptions:

Distributions All

- Prior \vec{x}_{k-1} , P_{k-1}
- Obs Unc R_k
- Temporal Evolution model Unc Q_{k-1}

are Gaussian

Models Both

- Observation Operator H
- Temporal Evolution model M

are linear

KF workings

Predict state

$$\vec{x}_{k|k-1} = \mathbf{M}_k^\top \vec{x}_{k-1|k-1} \quad \text{Advance state} \quad (22)$$

$$\mathbf{P}_{k|k-1} = \mathbf{M}_k^\top \mathbf{P}_{k-1|k-1} \mathbf{M}_k + \mathbf{Q}_k. \quad \text{Advance state uncert} \quad (23)$$

Ingest observations

$$\vec{r}_k = \vec{y}_k - \mathbf{H}_k \vec{x}_{k|k-1} \quad \text{Mismatch between prediction & Obs} \quad (24)$$

$$\mathbf{S}_k = \mathbf{H}_k^\top \mathbf{P}_{k|k-1} \mathbf{H}_k + \mathbf{R}_k. \quad \text{Innovation uncertainty} \quad (25)$$

State update

$$\mathbf{K}_k = \mathbf{P}_{k|k-1} \mathbf{H}_k \mathbf{S}_k^{-1}. \quad \text{Kalman gain} \quad (26)$$

$$\vec{x}_{k|k} = \vec{x}_{k|k-1} + \mathbf{K}_k \vec{r}_k. \quad \text{Update state conditioned on Obs} \quad (27)$$

$$\mathbf{P}_{k|k} = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k^\top) \mathbf{P}_{k|k-1}. \quad \text{Update state Unc conditioned on Obs} \quad (28)$$

Departures from the ideal case

A number of extensions to the standard KF have evolved to deal with non-idealities. These are:

Extended Kalman Filter (EKF) Deal with non-linearity by **linearising operators**.

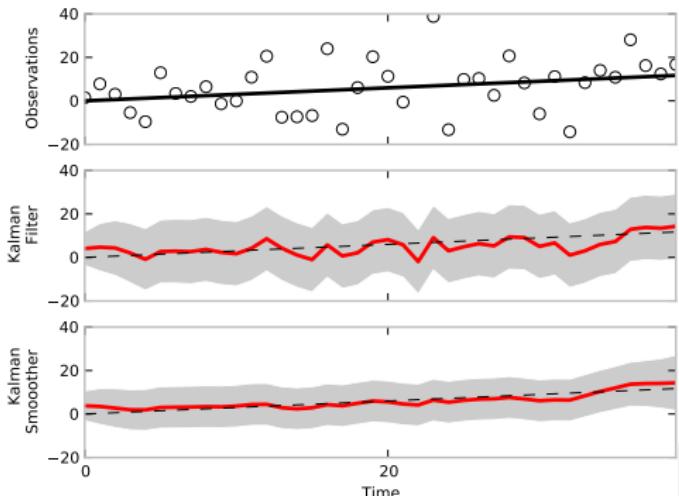
Ensemble Kalman Filter (EnKF) Run **an ensemble** of sample trajectories through the model.

Particle filter Monte Carlo method: uses a **finite number of particles** to represent the state. Lack of assumptions about linearity and normality.

Smoothers & Filters

- So far, we assume that we update the state synchronously from $k - 1$ to k to $k + 1$
- We could also update from $k + 1$ to k to $k - 1$
- For time step k , we have **two independent estimates** of the state, $\vec{x}_{k|k-1}$ and $\vec{x}_{k|k+1}$

- A **smoother** combines these two estimates
- Equivalent to a 4dVAR!

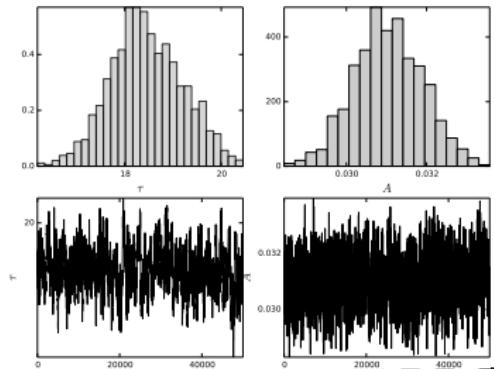
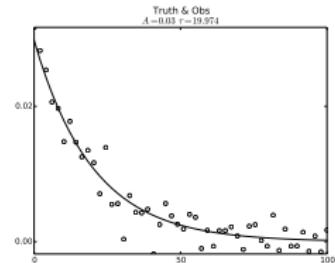


Sequential methods summary

- Kalman Filter: ideal for **linear** models and **normal** statistics
- (Extensions to KF to deal with non-linear models and non-normal stats)
- Main idea is to propagate state vector and uncertainty using a process model and use as prior for new observation assimilation
- Straightforward extension of the simple univariate case at the start!
- Smoothers: Combine fwd & bkwd KF to produce an equivalence to variational scheme

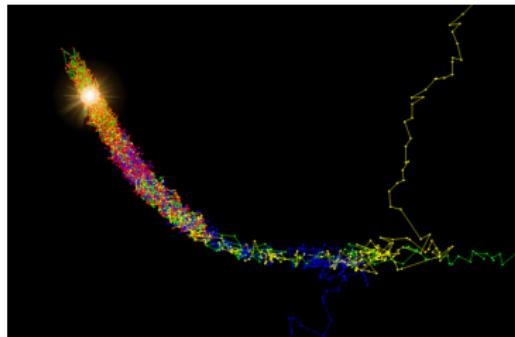
Markov Chain Monte Carlo (MCMC)

- No assumptions! Just solve whatever Bayesian problem you need by Monte Carlo sampling!
- Eg: measurements of exponential decay function
$$y_{obs} = A \exp [-t/\tau] + \epsilon_{obs}$$
- ... Solve for $p(A, \tau | y_{obs})$ using MCMC iterative approach and 50 000 iterations (!!)



MCMC comments

- Because of its lack of assumptions, MCMC is a general method to solve **inverse problems**
- You are guaranteed a solution, but this may require many iterations, so typically MCMC is painfully slow
- The algorithm is very simple, but more advanced & efficient versions exist
- MCMC might provide a benchmark solution to compare other algorithms and evaluate the effect of assumptions on DA performance.

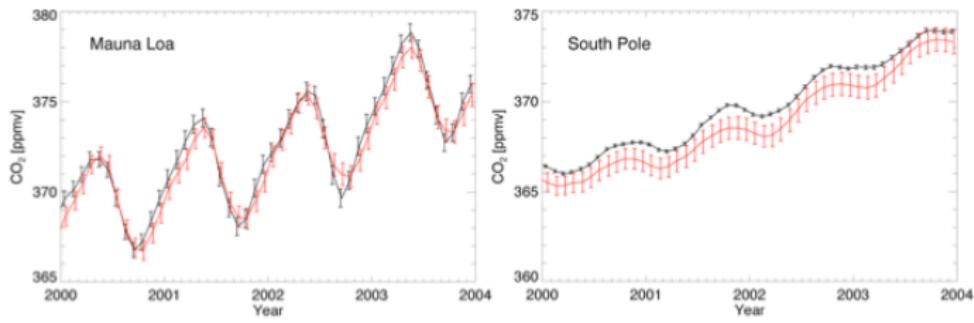


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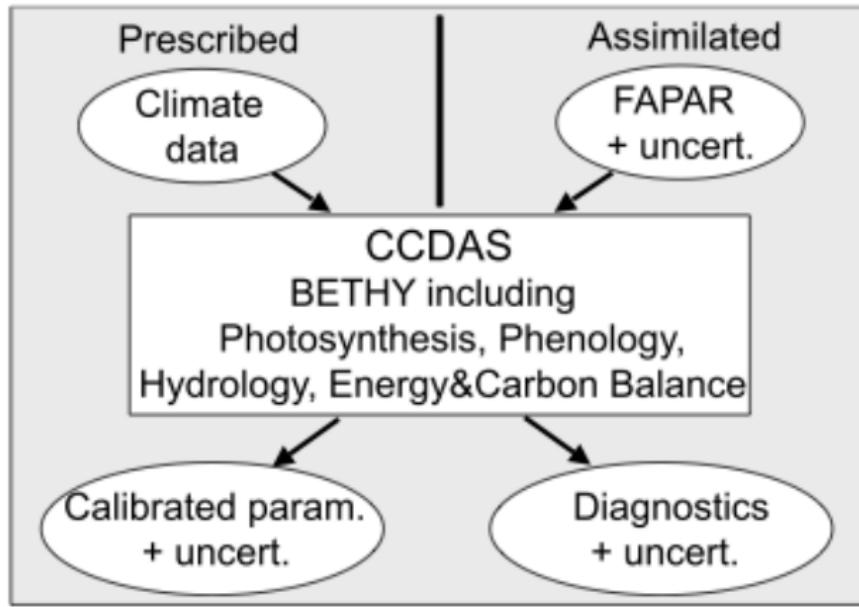
Carbon Cycle Data Assimilation System

- DA system around BETHY model (+partial derivs)
- Deal with e.g. atmospheric conc. data. Through coupled atmospheric tracer model
- Assimilate *fAPAR* and/or CO_2 concentrations



fAPAR assimilation

- Use *fAPAR* satellite-derived product
- $fAPAR \rightsquigarrow LAI$
- Predict CO_2 concentrations



fAPAR assimilation results

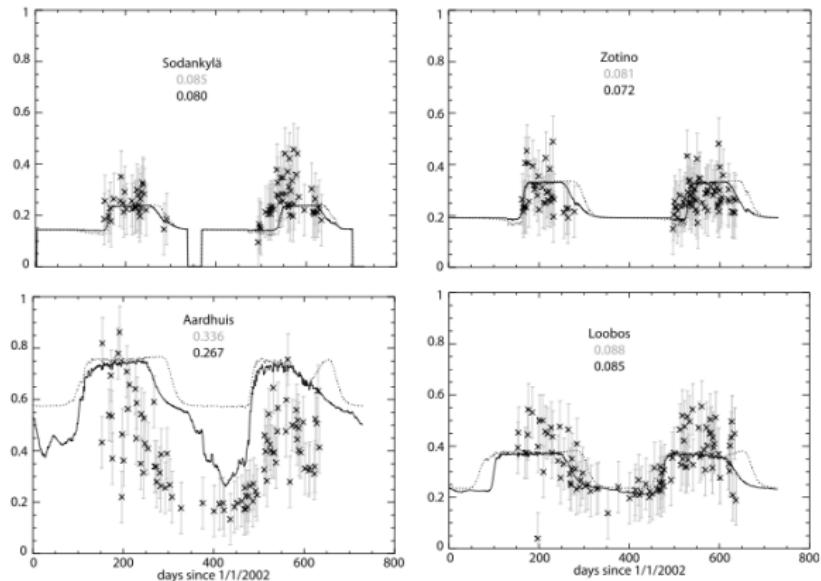


Figure 2. Observed (crosses with uncertainty ranges) and modeled prior (dotted) and posterior (solid line) FAPAR for Sodankylä, Zotino, Aardhuis, and Loobos from north to south. Numbers are root-mean-squared deviation between model and satellite data for the prior (gray) and posterior (black) case.

fAPAR assimilation results

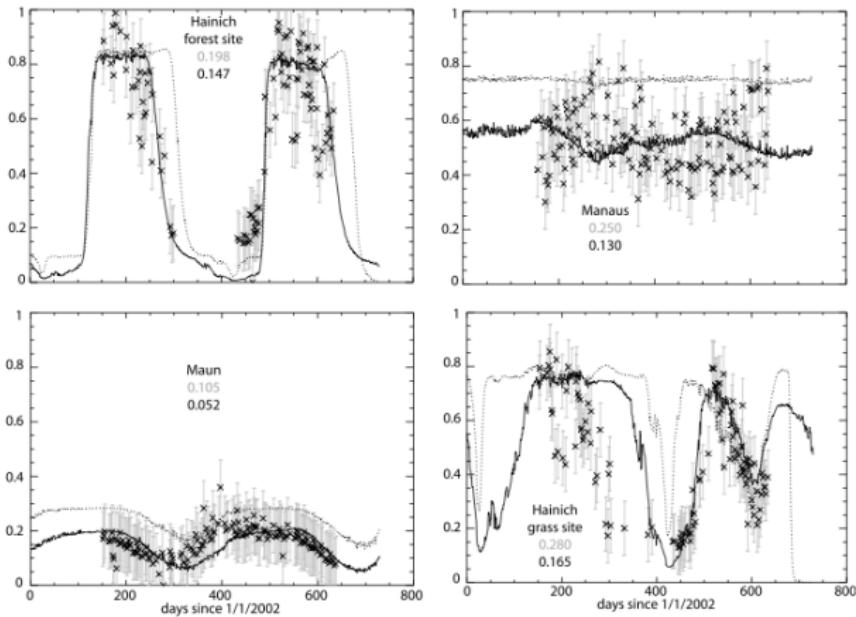


Figure 3. As in Figure 2, but for the Hainich forest site, Manaus, Maun, and the Hainich grass site. The Hainich grass site is shown for validation and not included in the assimilation.

fAPAR assimilation results

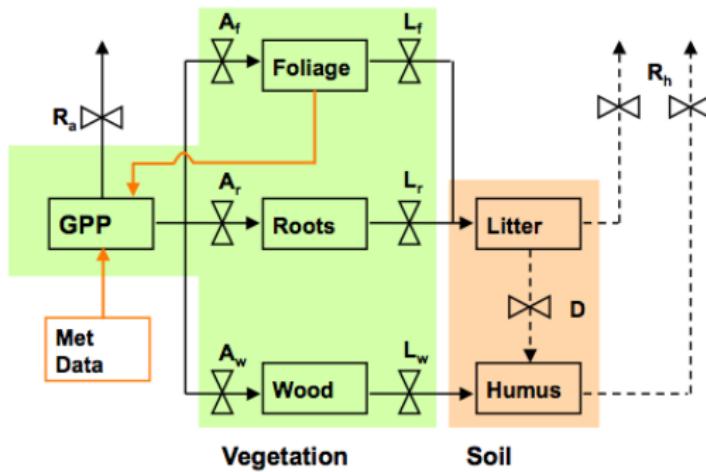
Table 7. Mean Annual Prior and Posterior NPP for the Period 2000–2003 (Inclusive) With Uncertainty, Change Relative to Prior Uncertainty, and Relative Uncertainty Reduction^a

Site			Relative Change (%)			Uncertainty Reduction (%)
	Prior NPP	Posterior NPP		Prior Uncertainty	Posterior Uncertainty	
Sodankylä	137	151	68	112	98	5
Zotino	201	216	54	28	28	0
Aardhuis	853	842	-7	164	101	38
Loobos	449	424	-40	62	59	5
Hainich forest	689	657	-29	112	98	13
Manaus	1465	964	-196	255	168	34
Maun	350	346	-10	50	46	8
Hainich grass	619	786	97	172	89	48

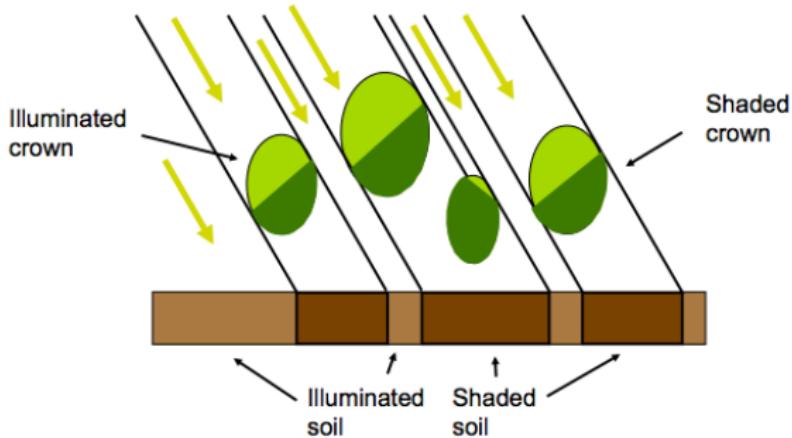
^aUnits are in $\text{gC m}^{-2} \text{ yr}^{-1}$ or percentage when stated.

EnKF & DALEC (Quaife *et al.*, 2008)

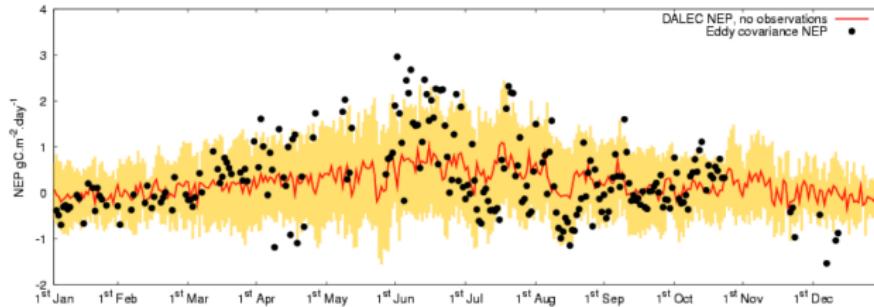
- It is hard to make e.g. *fAPAR* products consistent with radiative transfer in DGVMs
- Hard to track the noise on the product and how it feeds into the DA system
- So link the DGVM to the “raw” EO data (Surface Directional Reflectance, SDR)
- Need an (non-linear!) ObsOp to go from *LAI* to SDR



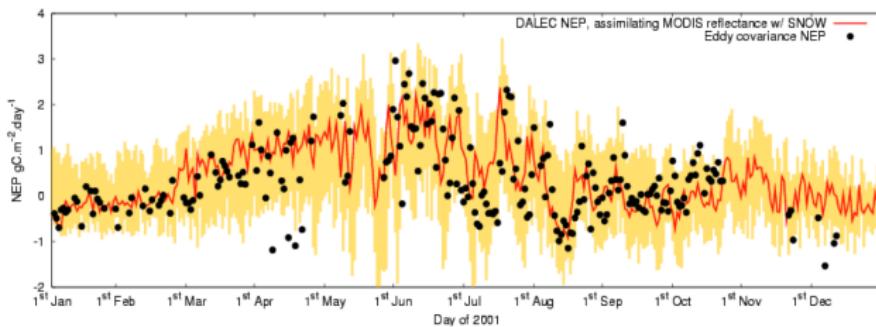
The ObsOp $\mathcal{H}(\vec{x})$



- Non-linear ObsOp \leadsto EnKF
- Observations constrain leaf C through LAI
- EO data requires information about other parameters
 - Leaf Chlorophyll concentration, soil reflectance, etc.
 - Assumed known and constant (!)



- Non-linear ObsOp \leadsto EnKF
- Observations constrain leaf C through *LAI*
- EO data requires information about other parameters
 - Leaf Chlorophyll concentration, soil reflectance, etc.
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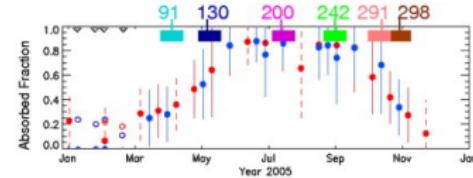
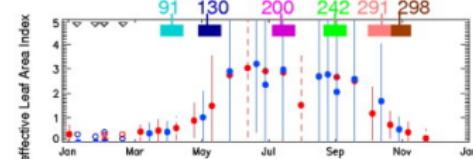
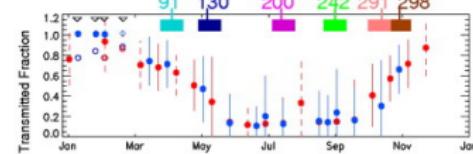


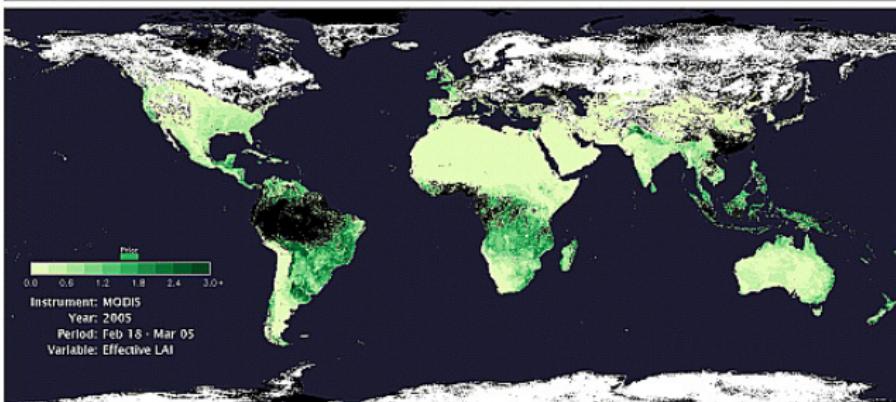
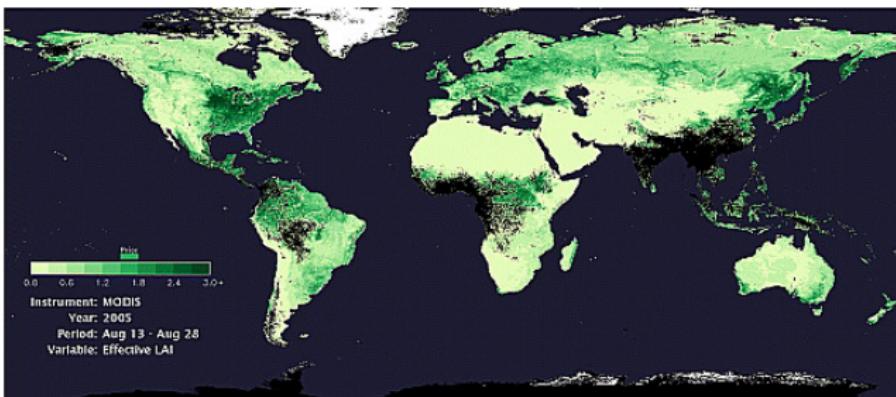
Results

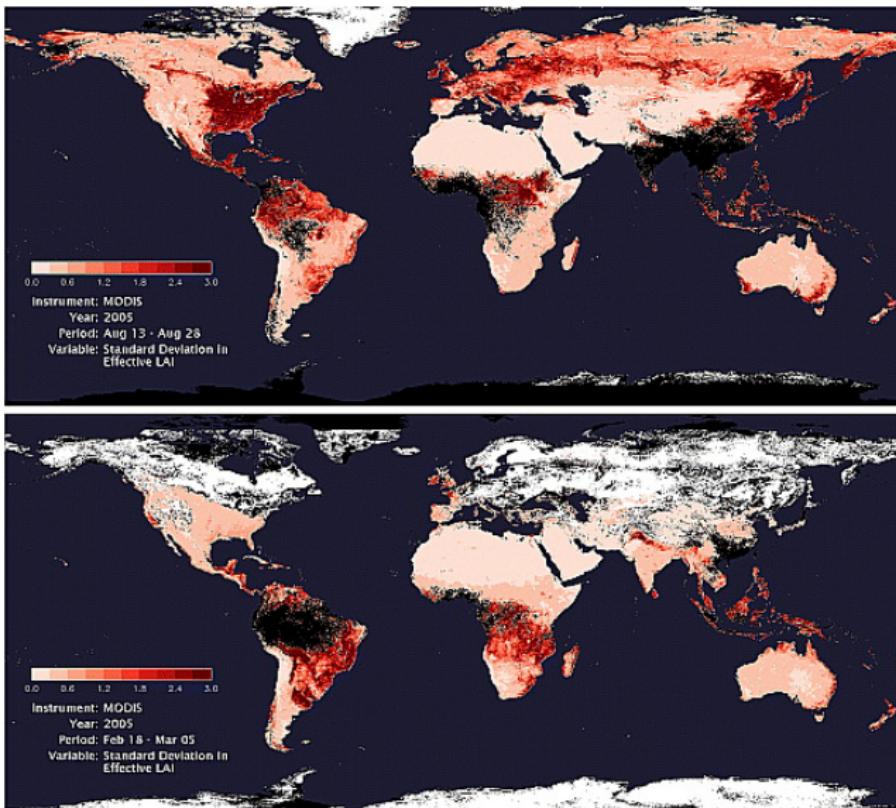
Flux (gC.m ⁻²)	Assimilated data	Total	Standard Deviation
NEP	Assimilation exc. snow	373.0	151.3
	Assimilation inc. snow	404.8	129.6
	Williams et al. (2005)	406.0	27.8
GPP	Assimilation exc. snow	2620.3	96.8
	Assimilation inc. snow	2525.6	42.7
	Williams et al. (2005)	2170.3	18.1

- Remember Bernard Pinty's seminar late last year?
- Use observations of **visible** and **near infrared albedo** from satellite to estimate radiative fluxes & LAI
- Variational scheme: prior on parameters & observations
- Use a fast and simple two stream RT model \rightsquigarrow effective LAI!
- Minimise $J(\vec{x})$ using partial derivatives
- Constant set of prior parameters for everywhere
- Each time step considered individually (i.e no temporal models)

$$\begin{aligned} J(\vec{x}) = & [\vec{x} - \vec{x}_0]^\top \mathbf{C}_0^{-1} [\vec{x} - \vec{x}_0] \\ & + [\alpha_{VIS} - \mathcal{H}(\vec{x})]^\top \mathbf{C}_{obs, VIS}^{-1} [\alpha_{VIS} - \mathcal{H}(\vec{x})] \\ & + [\alpha_{NIR} - \mathcal{H}(\vec{x})]^\top \mathbf{C}_{obs, NIR}^{-1} [\alpha_{NIR} - \mathcal{H}(\vec{x})] \end{aligned} \quad (29)$$

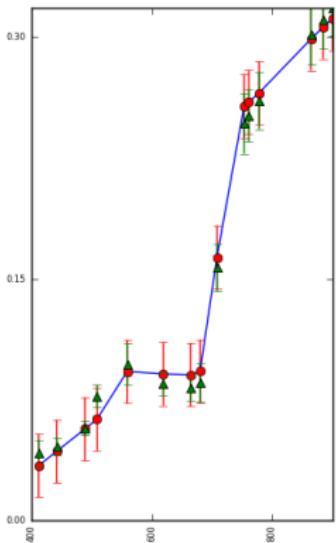






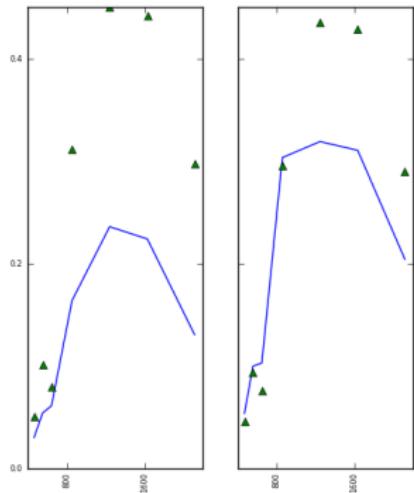
- Focus on interpreting EO data
- Simple models (temporal regularisation, i.e., prior on expectation of smooth parameter trajectory)
- Observation Operator: complex non-linear RT model + partial derivatives

Simple DA example



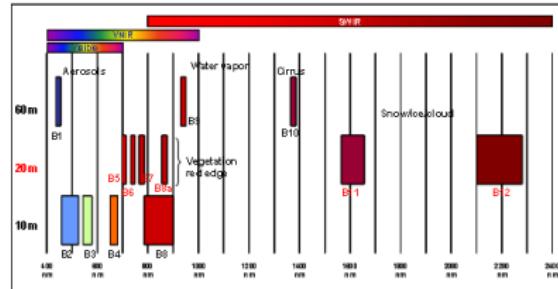
- From single MERIS observation
- Reduces uncertainty
- Models observation well
- Solve for 7 biophysical parameters here
- Uncertainty on most are high

Simple DA example



- Predict two MODIS obs on that same day
- Really poor performance!
- Ill-posed problems, remember?
- Strong correlation between parameters compensate fitting

EO-LDAS Sentinel-2 performance simulation



Spatial resolution 10m for bands in the VNIR, 60m for 3 atmosph correction bands, 20m other bands

Swath 290 km

Accuracy 3-5% absolute radiometric accuracy

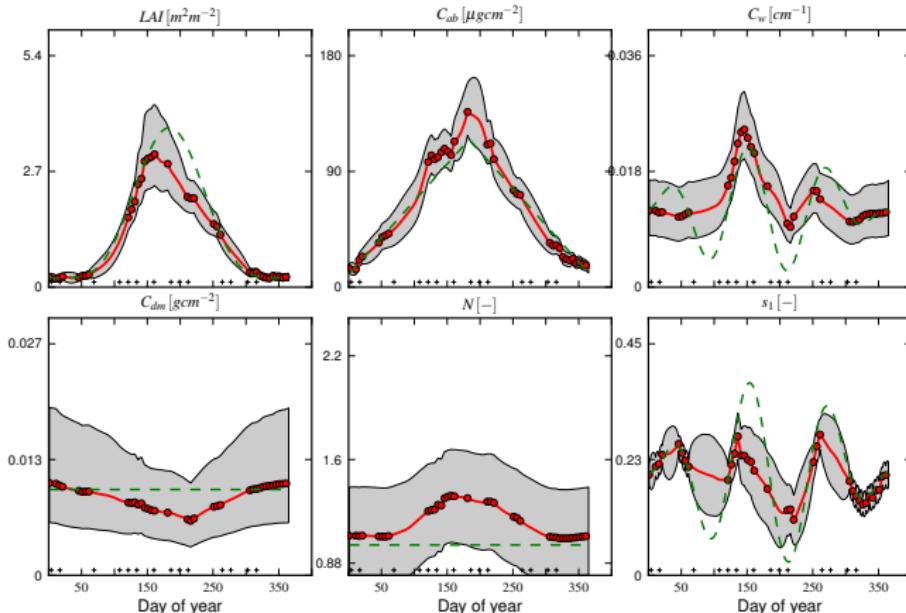
Wavelengths 13 in total, VIS, NIR & SWIR

Revisit period With 2 sensors, 5 days

Launch 2015?

S2 performance simulation

- Set of synthetic experiments, where land surface parameters are varied
- Simulate effect of cloudiness
- Use regularisation as temporal model (“*today same as yesterday, tomorrow same as today*”)



- CCDAS: practical example using complex models and satellite-derived products
- CCDAS drawbak: inconsistency between EO products and model?
Obs Uncertainty?
- Quaife et al: Solve previous point by assimilating reflectance directly
- JRC-TIP & EO-LDAS concentrate on EO
- JRC-TIP & EO-LDAS: variational systems
- EO-LDAS uses simple regularisation methods
- EO-LDAS is in
http://jgomezdans.github.com/jgomezdans/eoldas_ng

Outline

- 1 What is data assimilation (DA)?
- 2 From Bayes' Rule to DA
 - Assessing the update
- 3 DA methods
 - Variational schemes
 - Sequential methods: Filters & Smoothers
 - MCMC
- 4 Some DA examples
 - CCDAS
 - EnKF & DALEC model
 - JRC-TIP
 - EO-LDAS
- 5 Discussion

Summary

- State of the art quite basic (Use NDVI to calibrate phenology)
- CCDAS shows what can be achieved in a more consistent way
- JRC-TIP shows how to go about producing information about the land surface
- EO-LDAS shows a consistent way to use all available data to infer the state of the land surface
- Directly linking observations to models is a good idea as it simplifies uncertainty propagation
- However this is quite complex still!