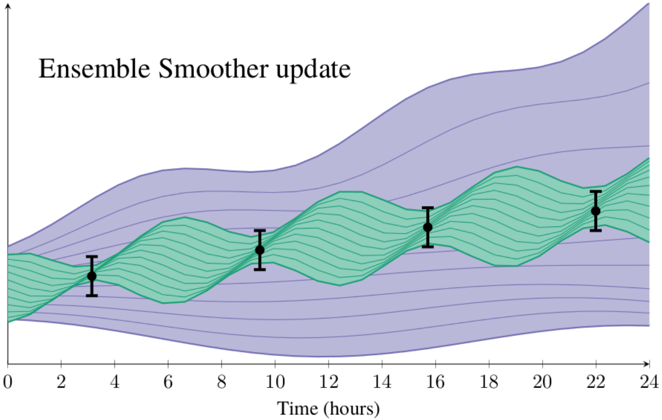
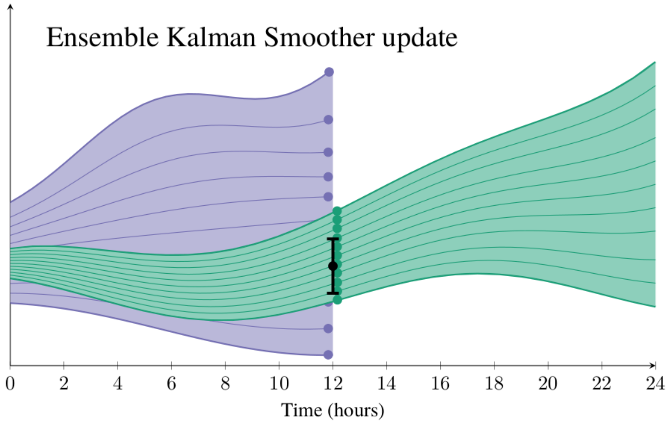
Using ensemble methods to solve inverse problems

Geir Evensen

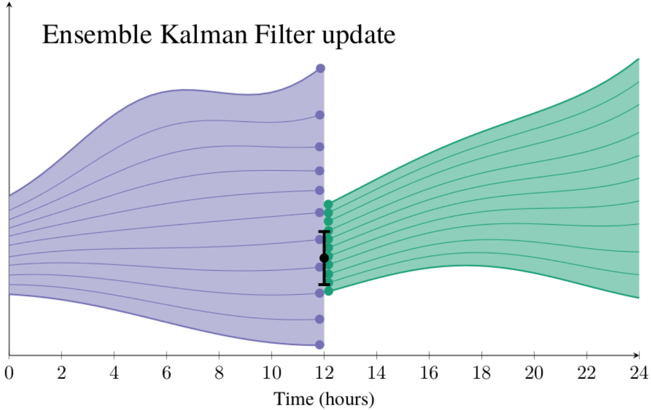
Ensemble Smoother (ES)



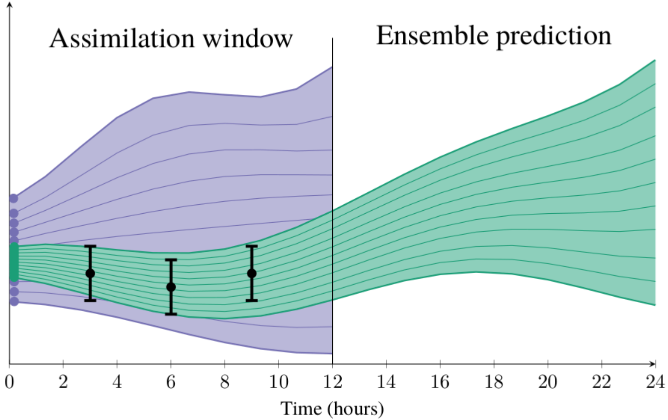
Ensemble Kalman Smoother (EnKS)



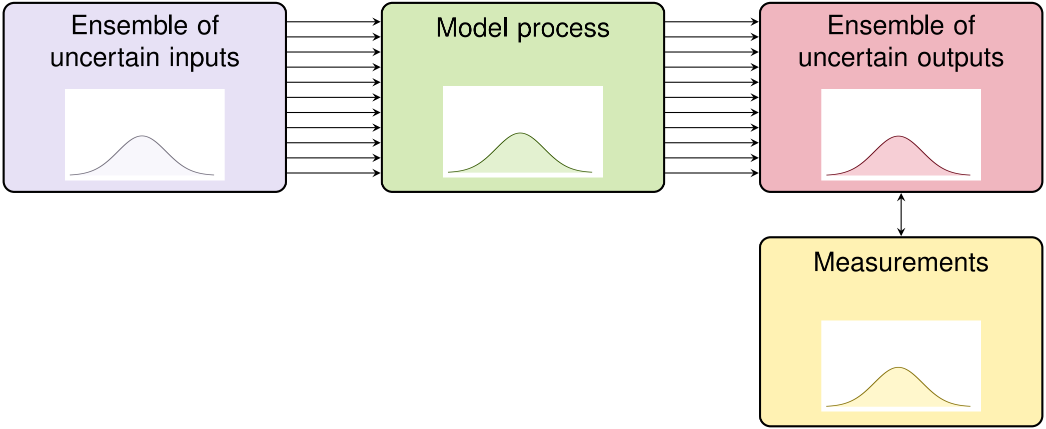
Ensemble Kalman Filter (EnKF)



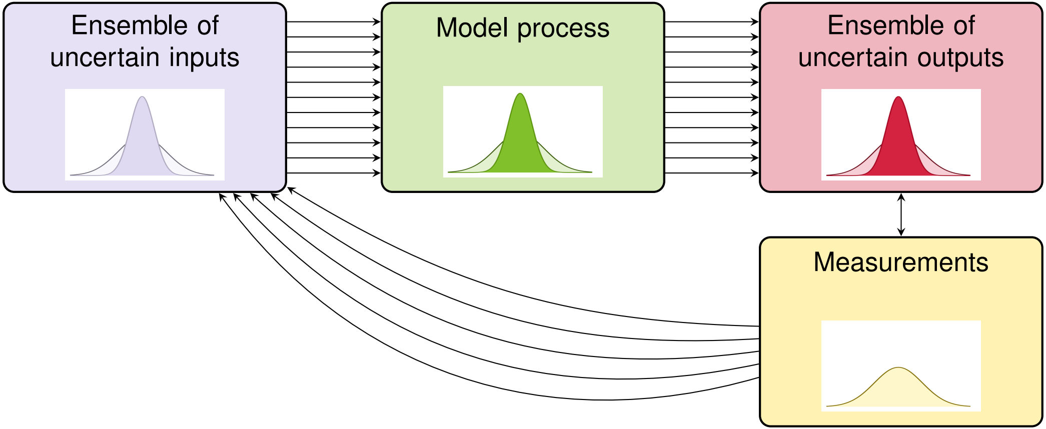
Ensemble DA for weather prediction



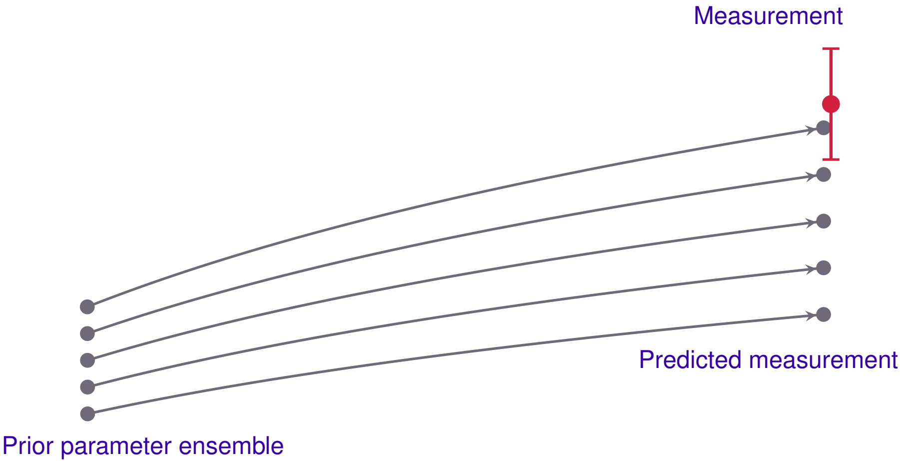
Ensemble DA for parameter estimation



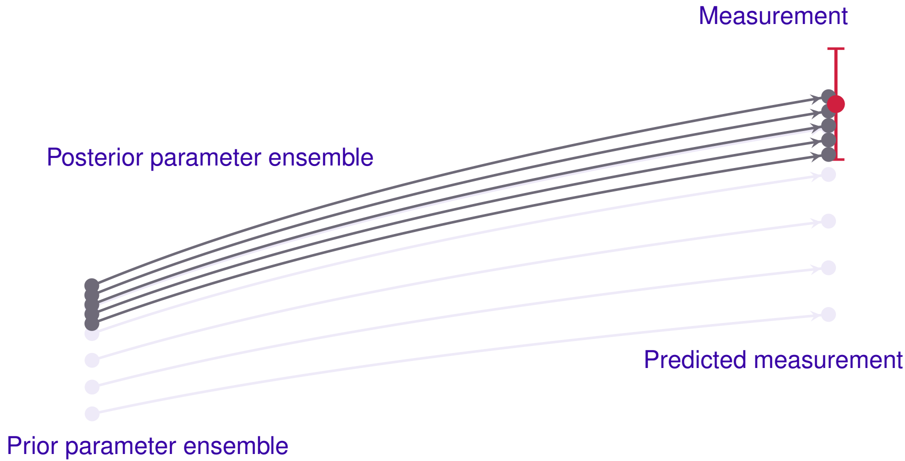
Ensemble DA for parameter estimation



Prior ensemble and measurement



Regression update using ensemble correlations



“Indirect” DA update

Nonlinear model

$$\boldsymbol{x}_{i+1} = \boldsymbol{m}(\boldsymbol{x}_i)$$

Nonlinear measurement operator and measurements

$$\boldsymbol{y} = \boldsymbol{h}(\boldsymbol{x}_{i+1}) = \boldsymbol{h}\big(\boldsymbol{m}(\boldsymbol{x}_i)\big) = \boldsymbol{g}(\boldsymbol{x}_i), \qquad \boldsymbol{d} \leftarrow \boldsymbol{y} + \boldsymbol{e}$$

Bayesian formulation

$$f(\boldsymbol{x}_i, \boldsymbol{y}|\boldsymbol{d}) \propto f(\boldsymbol{d}|\boldsymbol{y}) f(\boldsymbol{y}|\boldsymbol{x}_i) f(\boldsymbol{x}_i)$$

- Smoother update step in sequential data assimilation

Parameter-estimation problem

Nonlinear model and measurements

$$\boldsymbol{y} = \boldsymbol{g}(\boldsymbol{x}) \qquad \boldsymbol{d} \leftarrow \boldsymbol{y} + \boldsymbol{e}$$

Bayesian formulation

$$f(\boldsymbol{x}, \boldsymbol{y}|\boldsymbol{d}) \propto f(\boldsymbol{d}|\boldsymbol{y}) f(\boldsymbol{y}|\boldsymbol{x}) f(\boldsymbol{x})$$

- Standard Bayesian inverse problem

Deriving the marginal posterior pdf

Nonlinear "perfect" model and measurements

$$\boldsymbol{y} = \boldsymbol{g}(\boldsymbol{x}) \qquad \boldsymbol{d} \leftarrow \boldsymbol{y} + \boldsymbol{e}$$

Bayesian formulation

$$f(\boldsymbol{x}, \boldsymbol{y}|\boldsymbol{d}) \propto f(\boldsymbol{d}|\boldsymbol{y}) f(\boldsymbol{y}|\boldsymbol{x}) f(\boldsymbol{x})$$

Model pdf

$$f(\boldsymbol{y}|\boldsymbol{x}) = \delta\big(\boldsymbol{y} - \boldsymbol{g}(\boldsymbol{x})\big)$$

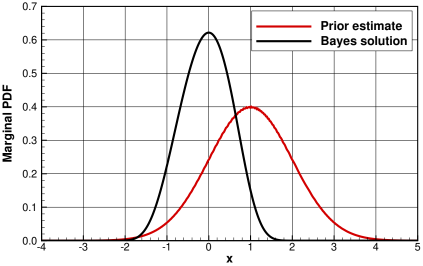
Marginal pdf

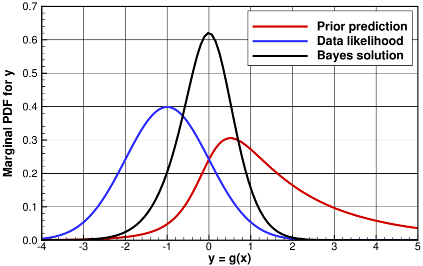
$$f(\boldsymbol{x}|\boldsymbol{d}) \propto \int f(\boldsymbol{d}|\boldsymbol{y}) f(\boldsymbol{y}|\boldsymbol{x}) f(\boldsymbol{x}) d\boldsymbol{y} = f\big(\boldsymbol{d}|\boldsymbol{g}(\boldsymbol{x})\big) f(\boldsymbol{x})$$

Illustration of the parameter estimation problem

Bayes theorem gives posterior probability function for parameters x

$$f(\boldsymbol{x}|\boldsymbol{d}) \propto f(\boldsymbol{d}\,|\,\boldsymbol{g}(\boldsymbol{x}))\,f(\boldsymbol{x})$$





Approximate sampling of the posterior pdf

Gaussian priors and randomized-maximum-likelihood sampling of

$$f(\boldsymbol{x}|\boldsymbol{d}) \propto f\big(\boldsymbol{d}\,|\,\boldsymbol{g}(\boldsymbol{x})\big)\, f(\boldsymbol{x})$$

by minimizing an ensemble of cost functions

$$\mathcal{J}(\boldsymbol{x}_j) = \underbrace{\big(\boldsymbol{x}_j - \boldsymbol{x}^{\mathrm{f}}_j\big)^{\mathrm{T}} \boldsymbol{C}_{xx}^{-1} \big(\boldsymbol{x}_j - \boldsymbol{x}^{\mathrm{f}}_j\big)}_{\text{Prior misfit}} \quad + \quad \underbrace{\big(\boldsymbol{g}(\boldsymbol{x}_j) - \boldsymbol{d}_j\big)^{\mathrm{T}} \boldsymbol{C}_{dd}^{-1} \big(\boldsymbol{g}(\boldsymbol{x}_j) - \boldsymbol{d}_j\big)}_{\text{data misfit}}.$$

Solutions methods:

1. Ensemble Smoother (ES) (van Leeuwen and Evensen, 1996) and (Evensen, 2009, Chap. 10).
2. Iterative Ensemble Smoother (IES) (Chen and Oliver, 2013).
3. Ensemble Smoother with Multiple Data Assimilation (ESMDA) (Emerick and Reynolds, 2013).

Ensemble Smoother

Approximately solves $\nabla \mathcal{J}_j = 0$

$$\boldsymbol{C}_{xx}^{-1}(\boldsymbol{x}_j - \boldsymbol{x}_j^{\mathrm{f}}) + \boldsymbol{G}_j^{\mathrm{T}} \boldsymbol{C}_{dd}^{-1} \big(\boldsymbol{g}(\boldsymbol{x}_j) - \boldsymbol{d}_j\big) = 0.$$

- Apply the linearization $\boldsymbol{g}(\boldsymbol{x}_j) = \boldsymbol{g}(\boldsymbol{x}_j^{\mathrm{f}}) + \boldsymbol{G}_j(\boldsymbol{x}_j - \boldsymbol{x}_j^{\mathrm{f}})$.
- Replace model sensitivities by least-squares fit $\boldsymbol{C}_{yx} = \boldsymbol{G}\boldsymbol{C}_{xx}$.
- ES uses ensemble covariances $\overline{\boldsymbol{C}}_{xy}$, $\overline{\boldsymbol{C}}_{xx}$, and $\overline{\boldsymbol{C}}_{dd}$.

$$\begin{aligned}
&\boldsymbol{x}_j^{\mathrm{f}} \leftarrow \mathcal{N}(\boldsymbol{x}^{\mathrm{f}}, \boldsymbol{C}_{xx}^{\mathrm{f}}), \qquad \boldsymbol{d}_j \leftarrow \mathcal{N}(\boldsymbol{d}, \boldsymbol{C}_{dd}),\\
&\boldsymbol{y}_j^{\mathrm{f}} = \boldsymbol{g}\big(\boldsymbol{x}_j^{\mathrm{f}}\big),\\
&\boldsymbol{x}_j^{\mathrm{a}} = \boldsymbol{x}_j^{\mathrm{f}} + \overline{\boldsymbol{C}}_{xy}\Big(\overline{\boldsymbol{C}}_{yy} + \overline{\boldsymbol{C}}_{dd}\Big)^{-1}\Big(\boldsymbol{d}_j - \boldsymbol{y}_j\Big),\\
&\boldsymbol{y}_j^{\mathrm{a}} = \boldsymbol{g}\big(\boldsymbol{x}_j^{\mathrm{a}}\big).
\end{aligned}$$

Iterative Ensemble Smoothers

State-space formulation with Gauss-Newton iterations

$$\mathcal{J}(\boldsymbol{x}_j) = \left(\boldsymbol{x}_j - \boldsymbol{x}_j^{\mathrm{f}}\right)^{\mathrm{T}} \boldsymbol{C}_{xx}^{-1} \left(\boldsymbol{x}_j - \boldsymbol{x}_j^{\mathrm{f}}\right) + \left(\boldsymbol{g}(\boldsymbol{x}_j) - \boldsymbol{d}_j\right)^{\mathrm{T}} \boldsymbol{C}_{dd}^{-1} \left(\boldsymbol{g}(\boldsymbol{x}_j) - \boldsymbol{d}_j\right)$$

with gradient and Hessian

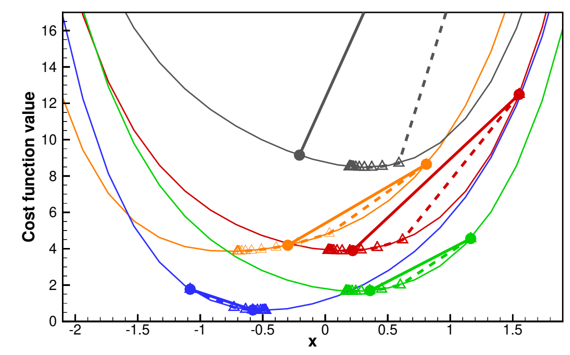
$$\nabla_x \mathcal{J} = \boldsymbol{C}_{xx}^{-1} \left(\boldsymbol{x}_j - \boldsymbol{x}_j^{\mathrm{f}}\right) + \boldsymbol{G}_j^{\mathrm{T}} \boldsymbol{C}_{dd}^{-1} \left(\boldsymbol{g}(\boldsymbol{x}_j) - \boldsymbol{d}_j\right),$$

$$\nabla_x \nabla_x \mathcal{J} \approx \boldsymbol{C}_{xx}^{-1} + \boldsymbol{G}_j^{\mathrm{T}} \boldsymbol{C}_{dd}^{-1} \boldsymbol{G}_j$$

Iterate

$$\begin{aligned} \boldsymbol{x}_j^{i+1} &= \boldsymbol{x}_j^{i} - \gamma \left(\nabla\nabla \mathcal{J}_i\right)^{-1} \nabla \mathcal{J}_j^{i} \\ \boldsymbol{y}_j^{i+1} &= \boldsymbol{g}\left(\boldsymbol{x}_j^{i+1}\right) \end{aligned}$$

ES and IES illustration: Non-linear model



- IES gets closer to minimum than ES
- Approximate sampling of posterior pdf.

ESMDA uses tempering of likelihood

Approximate sampling of $f(\boldsymbol{x}|\boldsymbol{d})$ by gradually introducing the measurements (Neal, 1996)

$$
\begin{aligned}
f(\boldsymbol{x}|\boldsymbol{d}) &= f(\boldsymbol{d}|\boldsymbol{y})\, f(\boldsymbol{x}) \\
&= f(\boldsymbol{d}|\boldsymbol{y})^{\left(\sum_{i=1}^{N} \frac{1}{\alpha_i}\right)} f(\boldsymbol{x}) \quad \text{with} \quad \sum_{i=1}^{N} \frac{1}{\alpha_i} = 1 \\
&= f(\boldsymbol{d}|\boldsymbol{y})^{\frac{1}{\alpha_N}} \cdots f(\boldsymbol{d}|\boldsymbol{y})^{\frac{1}{\alpha_2}} f(\boldsymbol{d}|\boldsymbol{y})^{\frac{1}{\alpha_1}} f(\boldsymbol{x})
\end{aligned}
$$

We compute N ES steps with “inflated” observation errors.

- Small updates reduce impact of the linear approximation.
- ESMDA is identical to ES in the linear case.
- Remember to resample measurement perturbations for each update step.

Some publications:

- Ensemble Randomized Maximum Likelihood EnRML (Chen and Oliver, 2013).
- Ensemble DA with multiple updates ESMDA (Emerick and Reynolds, 2013).
- Analysis of iterative ensemble smoothers (Evensen, 2018).
- IES with model errors (Evensen, 2019).
- Ensemble subspace RML (Evensen et al., 2019).

An international initiative of predicting the SARS-Cov-2 pandemic using ensemble data assimilation

http://www.aimsciences.org/article/doi/10.3934/fods.2021001

Geir Evensen

NORCE–Norwegian Research Center
Nansen Environmental and Remote Sensing Center

Colloquium seminar at IAC/ETH, March 8, 2021

American Institute of Mathematical Sciences

Title

Author

Home | Journals | Books | Conferences | News | Order | Contact

Previous Article | **FoDS** Home | This Issue | Next Article

doi: 10.3934/fods.2021001

An international initiative of predicting the SARS-CoV-2 pandemic using ensemble data assimilation

Geir Evensen [1], Javier Amezcua [2], Marc Bocquet [3], Alberto Carrassi [2,4], Alban Farchi [3], Alison Fowler [2], Pieter L. Houtekamer [5], Christopher K. Jones [6], Rafael J. de Moraes [7], Manuel Pulido [8], Christian Sampson [6] and Femke C. Vossepoel [7]

1. NORCE and NERSC, Bergen, Norway
2. Dept. of Meteorology University of Reading and NCEO, UK
3. CEREA, joint laboratory École des Ponts ParisTech and EDF R & D Université Paris-Est, Champs-sur-Marne, France
4. Mathematical Institute University of Utrecht, Netherlands
5. Environment and Climate Change Canada Dorval, Québec, Canada
6. Renaissance Computing Institute University of North Carolina, Chapel Hill, USA
7. Department of Geoscience and Engineering Delft University of Technology, Delft, Netherlands
8. FaCENA, UNNE and IMIT, CONICET Corrientes, Argentina

Available observations

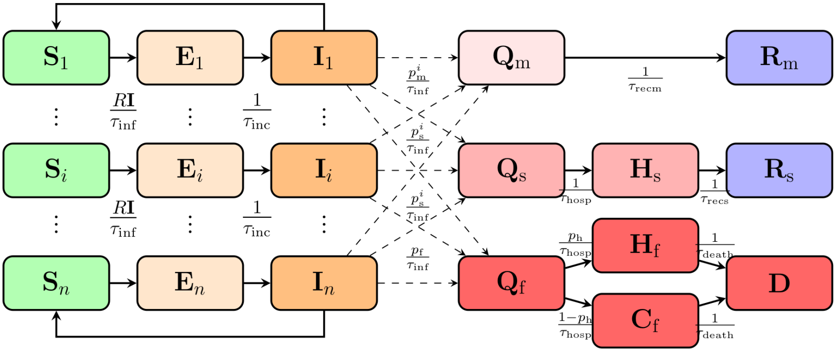
Hospitalized: Within different agegroups and gender.

Deaths: At hospitals or care homes.

Cases: Positive tests (highly underreported).

1. Data uncertainty and availability varies in different countries.
2. The SEIR model doesn't predict deaths and hospitalizations.

Extended SEIR model



- We add age classes to model age-specific infection and death rates.
- We differentiate between mild, severe, and fatal symptoms.
- We model those with fatal symptoms who die in care homes.

Extended SEIR model

$$\frac{\partial \boldsymbol{S}_i}{\partial t} = -\left(\sum_{j=1}^{n} \frac{R_{ij}(t)\boldsymbol{I}_j}{\tau_{\text{inf}}}\right)\boldsymbol{S}_i \tag{1}$$

$$\frac{\partial \boldsymbol{E}_i}{\partial t} = \left(\sum_{j=1}^{n} \frac{R_{ij}(t)\boldsymbol{I}_j}{\tau_{\text{inf}}}\right)\boldsymbol{S}_i - \frac{1}{\tau_{\text{inc}}}\boldsymbol{E}_i \tag{2}$$

$$\frac{\partial \boldsymbol{I}_i}{\partial t} = \frac{1}{\tau_{\text{inc}}}\boldsymbol{E}_i - \frac{1}{\tau_{\text{inf}}}\boldsymbol{I}_i \tag{3}$$

$$\frac{\partial \boldsymbol{Q}_{\text{m}}}{\partial t} = \sum_{i=1}^{n} \frac{p_{\text{m}}^i}{\tau_{\text{inf}}}\boldsymbol{I}_i - (1/\tau_{\text{recm}})\boldsymbol{Q}_{\text{m}} \tag{4}$$

$$\frac{\partial \boldsymbol{Q}_{\text{s}}}{\partial t} = \sum_{i=1}^{n} \frac{p_{\text{s}}^i}{\tau_{\text{inf}}}\boldsymbol{I}_i - (1/\tau_{\text{hosp}})\boldsymbol{Q}_{\text{s}} \tag{5}$$

$$\frac{\partial \boldsymbol{Q}_{\text{f}}}{\partial t} = \sum_{i=1}^{n} \frac{p_{\text{f}}^i}{\tau_{\text{inf}}}\boldsymbol{I}_i - (1/\tau_{\text{hosp}})\boldsymbol{Q}_{\text{f}} \tag{6}$$

$$\frac{\partial \boldsymbol{H}_{\text{s}}}{\partial t} = \frac{1}{\tau_{\text{hosp}}}\boldsymbol{Q}_{\text{s}} - \frac{1}{\tau_{\text{recs}}}\boldsymbol{H}_{\text{s}} \tag{7}$$

$$\frac{\partial \boldsymbol{H}_{\text{f}}}{\partial t} = \frac{p_{\text{h}}}{\tau_{\text{hosp}}}\boldsymbol{Q}_{\text{f}} - \frac{1}{\tau_{\text{death}}}\boldsymbol{H}_{\text{f}} \tag{8}$$

$$\frac{\partial \boldsymbol{C}_{\text{f}}}{\partial t} = \frac{(1-p_{\text{h}})}{\tau_{\text{hosp}}}\boldsymbol{Q}_{\text{f}} - \frac{1}{\tau_{\text{death}}}\boldsymbol{C}_{\text{f}} \tag{9}$$

$$\frac{\partial \boldsymbol{R}_{\text{m}}}{\partial t} = \frac{1}{\tau_{\text{recm}}}\boldsymbol{Q}_{\text{m}} \tag{10}$$

$$\frac{\partial \boldsymbol{R}_{\text{s}}}{\partial t} = \frac{1}{\tau_{\text{recs}}}\boldsymbol{H}_{\text{s}} \tag{11}$$

$$\frac{\partial \boldsymbol{D}}{\partial t} = \frac{1}{\tau_{\text{death}}}\boldsymbol{H}_{\text{f}} + \frac{1}{\tau_{\text{death}}}\boldsymbol{C}_{\text{f}} \tag{12}$$

Validity of the SEIR model

- Aggregated variables (statistical significance).
- Neglects import of cases (ok during lockdown).
- SEIR type models tend to successfully model epidemics.
- The simplicity is a huge advantage.

More complex models involve additional parameters.

Constant model parameters

1. Relative fractions p^i_{m}, p^i_{s}, p^i_{f} per age group.
2. Fractions dying in a Hospital p_{h} versus in a Care home $1 - p_{\mathrm{h}}$.

Age group	1	2	3	4	5	6	7	8	9	10	11
Age range	0–5	6–12	13–19	20–29	30–39	40–49	50–59	60–69	70–79	80–89	90–105
p–mild	1.00	1.00	0.99	0.99	0.97	0.96	0.93	0.90	0.84	0.81	0.81
p–severe	0.00	0.00	0.00	0.00	0.02	0.02	0.05	0.08	0.11	0.11	0.11
p–fatal	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.06	0.06

Model parameters estimated by DA

Parameter	First guess	Description
τ_{inc}	5.5	Incubation period
τ_{inf}	3.8	Infection time
τ_{recm}	14.0	Recovery time mild cases
τ_{recs}	5.0	Recovery time severe cases
τ_{hosp}	6.0	Time until hospitalization
τ_{death}	16.0	Time until death
p_{f}	0.009	Case fatality rate
p_{s}	0.039	Hospitalization rate (severe cases)
I_0		Initial number of infectious
E_0		Initial number of exposed
$R(t)$		Effective reproductive number

Effective reproductive number

$$\boldsymbol{R}(t) = R(t)\hat{\boldsymbol{R}}$$

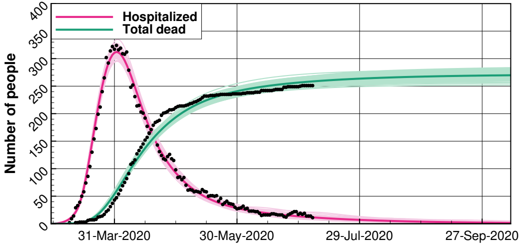
$\boldsymbol{R}(t)$ is a function of time (steered by how people isolate or interact).

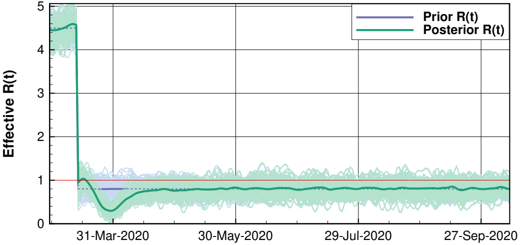
- $R(t)$ is a scalar function of time.
- $\hat{\boldsymbol{R}}$ a constant matrix of transmissions between age classes..
- Behavior two weeks ago determines today's deaths and hospitalizations.
- We can estimate $R(t)$ for the past.
- We assume the value $R(t)$ for the future.

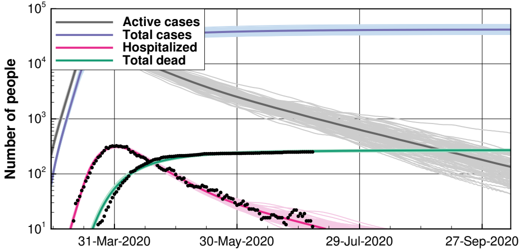
We used ESMDA

- Simple implementation and use.
- Efficient for large ensemble sizes.
- 5000 realizations and 32 ESMDA steps.

Example from Norway

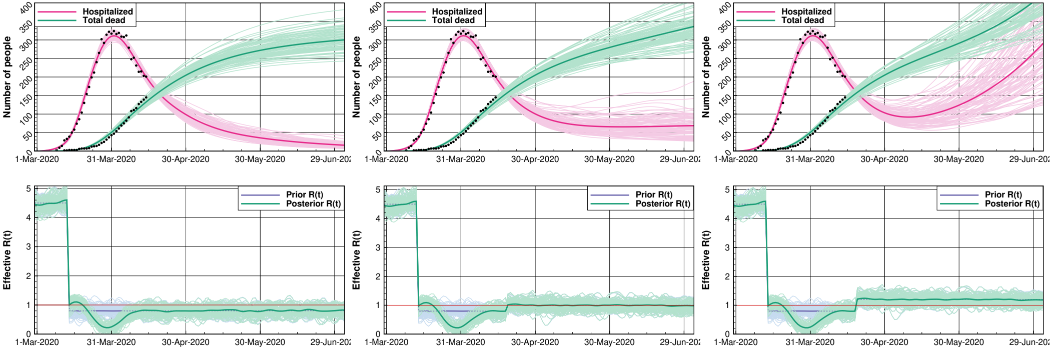




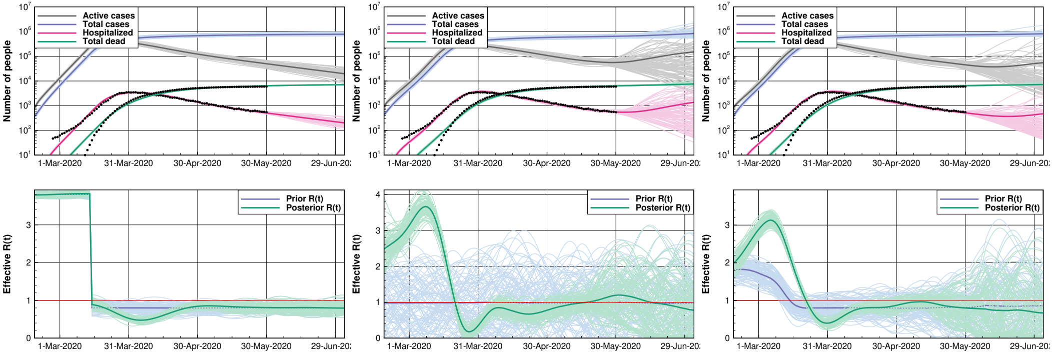


NORCE

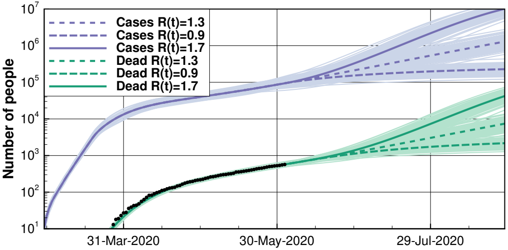
Back-to-school scenarios for Norway

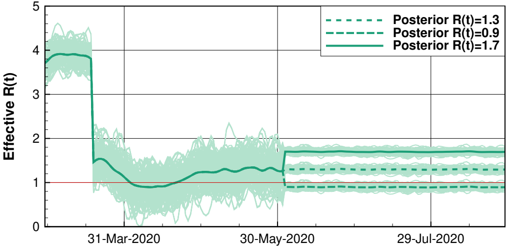


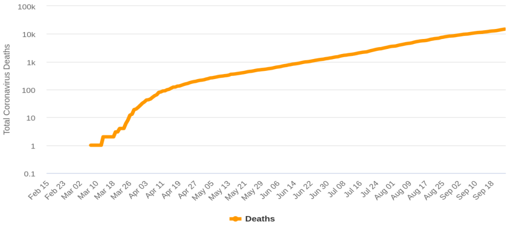
$R(t)$ example: The Netherlands



Scenarios: Argentina

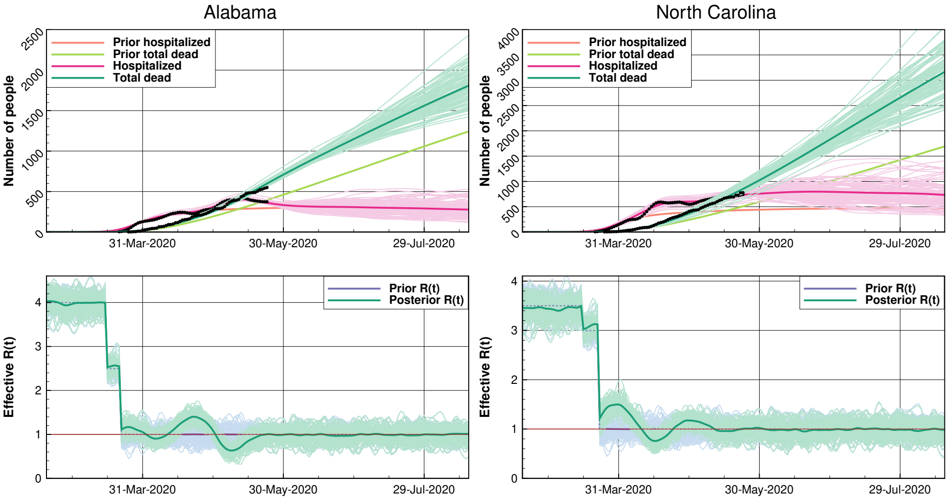




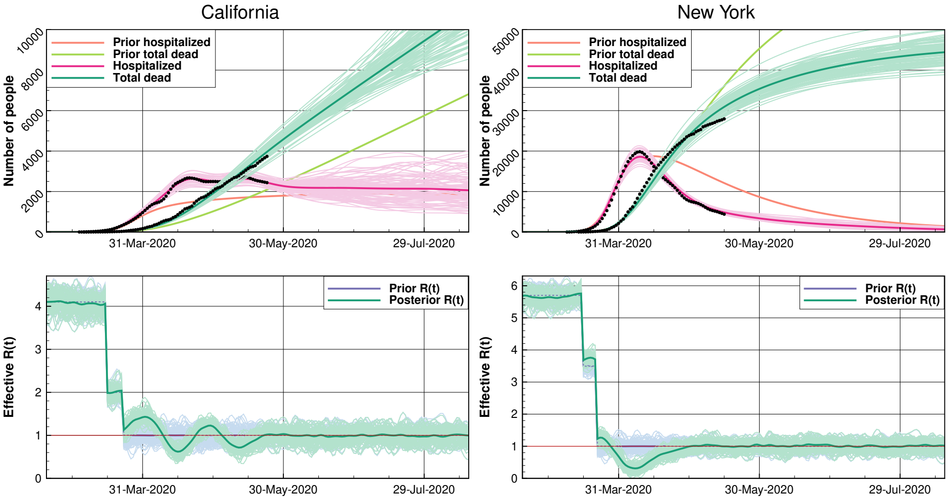


8660 deaths and 417000 cases at Aug 31.

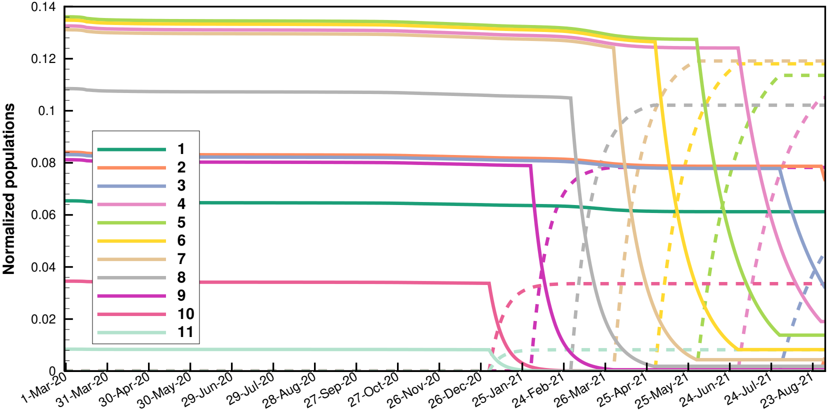
US: Modeling time variability in $R(t)$



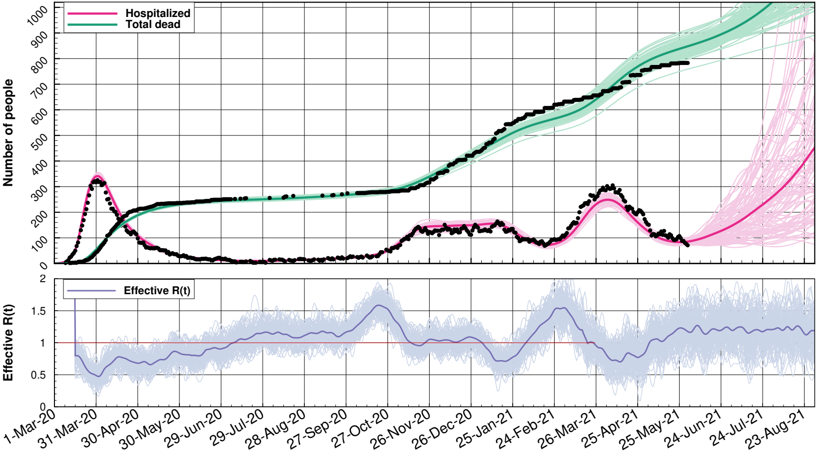
US: Modeling time variability in $R(t)$



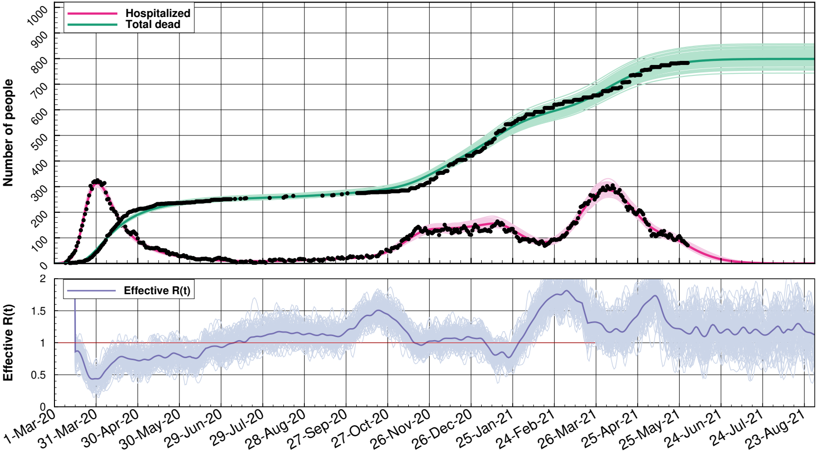
Norway: Vaccination prediction



Norway: prediction without vaccinations



Norway: prediction with vaccinations



Summary EnKF_seir

- The DA system tracks the epidemic accurately.
- We can estimate past $R(t)$.
- It is possible to quantify the impact of interventions.
- Short-term forecasting using R-persistence works well.
- Long-term scenario forecasting with specified future R.
- Code: https://github.com/geirev/EnKF_seir
- Paper: (Evensen et al., 2020)
  http://www.aimsciences.org/article/doi/10.3934/fods.2021001

Outlook EnKF_seir

- The code now supports multiple countries that interact.
- Study general dynamics of multi-populations under different intervention regimes.
- Inclusion of a term compensation for vacination.
- Impact of new mutated viruses with different R(t).
- Simulating reopening strategies accounting for mutations and vaccinations.

Bibliography

Chen, Y. and D. S. Oliver. Levenberg-Marquardt forms of the iterative ensemble smoother for efficient history matching and uncertainty quantification. *Computat Geosci*, 17:689–703, 2013. doi:10.1007/s10596-013-9351-5.

Emerick, A. A. and A. C. Reynolds. Ensemble smoother with multiple data assimilation. *Computers and Geosciences*, 55:3–15, 2013. doi:10.1016/j.cageo.2012.03.011.

Evensen, G. *Data Assimilation: The Ensemble Kalman Filter*. Springer, 2nd edition, 2009. doi:10.1007/978-3-642-03711-5.

Evensen, G. Analysis of iterative ensemble smoothers for solving inverse problems. *Computat Geosci*, 22(3):pp. 885–908, 2018. doi:10.1007/s10596-018-9731-y.

Evensen, G. Accounting for model errors in iterative ensemble smoothers. *Computat Geosci*, 23(4):pp. 761–775, 2019. doi:10.1007/s10596-019-9819-z.

Evensen, G., P. Raanes, A. Stordal, and J. Hove. Efficient implementation of an iterative ensemble smoother for data assimilation and reservoir history matching. *Frontiers in Applied Mathematics and Statistics*, 5:47, 2019. doi:10.3389/fams.2019.00047.

Evensen, G., J. Amezcua, M. Bocquet, A. Carrassi, A. Farchi, A. Fowler, P. L. Houtekamer, C. K. Jones, R. J. de Moraes, M. Pulido, C. Sampson, and F. C. Vossepoel. An international initiative of predicting the sars-cov-2 pandemic using ensemble data assimilation. *Foundations of Data Science*, page 65, 2020. doi:10.3934/fods.2021001.

Neal, R. M. Sampling from multimodal distributions using tempered transitions. *Statistics and Computing*, 6(4):353–366, 1996. doi:10.1007/BF00143556.

van Leeuwen, P. J. and G. Evensen. Data assimilation and inverse methods in terms of a probabilistic formulation. *Mon. Weather Rev.*, 124:2898–2913, 1996. doi:10.1175/1520-0493(1996)124<2898:DAAIMI>2.0.CO;2.