Forecasting Ozone at European Scale with Ensembles

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Research carried out in the INRIA-ENPC joint project-team CLIME

and in the ENPC-EDF R&D joint laboratory CEREA

Motivations

Limitations of Deterministic Approches

- High uncertainties: input data, parameterizations, numerical resolution, even bugs and user mistakes
- State dimension, 10^6–10^7, versus number of observations, 10^2
- (Over)tuning ?
- A single forecast, even the best one, is uncertain

Ensemble Approaches to Overtake Uncertainties

- Several models bring more information
- From *all-in-one* models to a *platform of model configurations*
  - Fragmented model: Alternative physical formulations
Alternative numerical schemes
Alternative input data
  - A model configuration may be viewed as a new model

Building a Multimodel Ensemble

Tool: the Air Quality Modeling System Polyphemus

- Ancient Greek: “multiple speeches”
- See the poster (design and contents of Polyphemus)

Mallet, Quélo, Sportisse, Ahmed de Biasi, Debry, Korsakissok, Wu, Roustan, Sartelet, Tombette and Foudhil, *Technical Note: The air quality modeling system Polyphemus*, ACPD, 2007

Ensemble Capabilities

- Used in current work
  - Alternative physical parameterizations
  - Several input data sources
  - Numerical modules
- Not used for the moment
  - Two “base” Eulerian chemistry-transport models
  - Model coupling (plume-in-grid, nesting)
  - Data assimilation algorithms (OI, Kalman filters, 4D-Var)

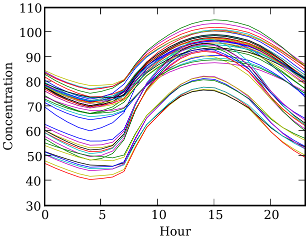
Building a Multimodel Ensemble (cont.)

#	*Parameterization*	*Reference*	*Alternative(s)*
		Physical parameterizations	
1.	Chemistry	RACM	RADM 2
2.	Vertical diffusion	Troen & Mahrt	Louis
3.			Louis in stable conditions
4.	Deposition velocities	Zhang	Wesely
5.	Surface flux	Heat flux	Momentum flux
6.	Cloud attenuation	RADM method	Esquif
7.	Critical relative humidity	Depends on σ	Two layers
		Input data	
8.	Emissions vertical distribution	All in the first cell	All in the two first cells
9.	Land use coverage (dep.)	USGS	GLCF
10.	Land use coverage (bio.)	USGS	GLCF
11.	Exponent p in Troen & Mahrt	2	3
12.	Photolysis rates	JPROC	Depends on zenith angle
		Numerical issues	
13.	Time Step	600 s	100 s
14.			1800 s
15.	Splitting method	First order	Strang splitting
16.	Horizontal resolution	0.5°	0.1°
17.			1.0°
18.	Vertical resolution	5 layers	9 layers
19.	First layer height	50 m	40 m

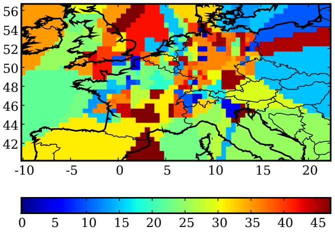
Ensemble Simulations Bring Useful Information

Study

- Ozone simulations at European scale during 4 months
- Resolution of 0.5°, 5 layers up to 3000 m
- ECMWF meteorological fields
- 48 members in the ensemble



Ozone daily profiles from 48 members



Best model index

Best Model and Ensemble Mean Are Limited

Model Combination and Advanced Methods Are Desirable

Notations

Output of model m at time t and position x: $M_{m,t,x}$

Linear combination: $E_{t,x} = \sum_m \alpha_{m,t} M_{m,t,x}$

Observation: $O_{t,x}$

Best Model: the Reference to Improve

- $EB_{t,x} = M_{\widehat{m},t,x}$ where $\widehat{m}$ minimizes $\mathrm{RMSE}(M_m, O)$
- $\mathrm{RMSE}(EB, O) = 22.4\ \mu\mathrm{g\,m^{-3}}$

Ensemble Mean: the Most Simple Combination

- $EM_{t,x} = \overline{M_{m,t,x}}^{m}$
- $\mathrm{RMSE}(EM, O) = 23.9\ \mu\mathrm{g\,m^{-3}}$

Conclusion: “assimilation” of observations is needed

Combining Models

Least-Squares Methods or “Superensembles” (Krishnamurti et al., 2000)

Potential: *A Posteriori* Coefficients

- $ELS_{t,x} = \sum_m \alpha_{m,t} M_{m,t,x}$ where
  $\forall t \quad \alpha_{\cdot,t} = \mathrm{argmin} \sum_x \left(O_{t,x} - \sum_m \alpha_{m,t} M_{m,t,x}\right)^2$
- $\mathrm{RMSE}(ELS, O) = 12.0\ \mu\mathrm{g\,m^{-3}}$ (best model: $22.4\ \mu\mathrm{g\,m^{-3}}$)

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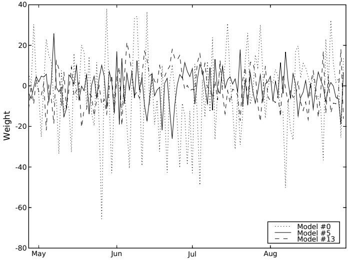

Time evolution of optimal weights (*ELS*)

Combining Models

Least-Squares Methods or “Superensembles” (Krishnamurti et al., 2000)

Smoothing Weights Time Evolution and Forecasting

- $ELS^{30}_{t,x} = \sum_m \alpha^{30}_{m,t} M_{m,t,x}$ where
  $\forall t \quad \alpha^{30}_{\cdot,t} = \text{argmin} \sum_{t-30 \leq T < t,x} \left(O_{T,x} - \sum_m \alpha_{m,T} M_{m,T,x}\right)^2$
- $\text{RMSE}(ELS^{30}, O) = 20.2\ \mu\text{g m}^{-3}$ (againt $22.4\ \mu\text{g m}^{-3}$)

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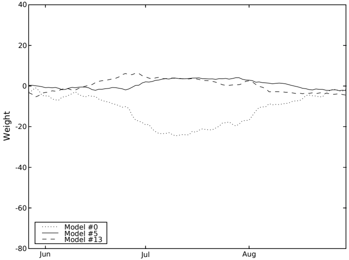

Time Evolution of Forecast Weights (ELS^{30})

Example: Exponentiated Gradient (Kivinen and Warmuth, 1997)

- Combination $EG_{t,x} = \sum_m \alpha_{m,t} M_{m,t,x}$
- Loss function: $L(EG_{t,\cdot}, O_{t,\cdot}) = \sum_x (EG_{t,x} - O_{t,x})^2$
- Weights update:

$$\forall m \quad \alpha_{m,t+1} = \exp\left(-\eta \frac{\partial L(EG_{t,\cdot}, O_{t,\cdot})}{\partial \alpha_{m,t}}\right) \times \text{normalization}$$

- Choice: learning rate η
- Bound on the regret $\left|\sum_t L(EG_{t,\cdot}, O_{t,\cdot}) - \min_\alpha \sum_t L(\sum_m \alpha_m M_{m,t,\cdot}, O_{t,\cdot})\right| \leq \gamma N_{\text{station}} \sqrt{N_{\text{step}} \ln N_{\text{model}}}$
- $\text{RMSE}(EG\,(\eta = 10^{-5}), O) = 21.6\ \mu\text{g}\,\text{m}^{-3}$

Hybrid Methods

Joint Work with Gilles Stoltz (CNRS; ENS Paris)

Hybrid Method

- Purpose: join performances of ELS^{30} and theoretical bounds from learning algorithms
- Strategy: include ELS^{30} (and possibly other combinations) in the ensemble, and apply learning (meta-)algorithm

Example

- Ensemble: 48 models plus ELS^{30}, ELS^{20} and ELS^{10}
- Learning algorithm: extended exponential gradient, with $\eta = 10^{-5}$
- Successful result: 19.9 $\mu g\, m^{-3}$

Conclusions

- Ensemble forecast relying on Polyphemus design
  - *Technical Note: The air quality modeling system Polyphemus*, Mallet, Quélo, Sportisse, Ahmed de Biasi, Debry, Korsakissok, Wu, Roustan, Sartelet, Tombette and Foudhil, ACPD, 2007
- Detailed uncertainty analysis (not shown here)
  - *Uncertainty in a chemistry-transport model due to physical parameterizations and numerical approximations: An ensemble approach applied to ozone modeling*, Mallet & Sportisse, JGR, 2006
- Model sequential aggregation to improve forecasts
  - *Ensemble-based air quality forecasts: a multimodel approach applied to ozone*, Mallet & Sportisse, JGR, 2006
  - *Ozone ensemble forecast with machine learning algorithms*, Mallet & Stoltz, in preparation
- Toward operational use
  - 43 models ran every day with Prév'air data, for 4 months in 2006 – but without aggregation