École Doctorale des Sciences de l'Environnement d'Île-de-France

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Modélisation Numérique de l'Écoulement Atmosphérique et Assimilation de Données

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Cours 3

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Bayesian Estimation

Determine conditional probability distribution of the state of the system, given the probability distribution of the uncertainty on the data

$$z_1 = x + \zeta_1 \qquad \zeta_1 = \mathcal{N}[0, s_1]$$

density function $p_1(\zeta) \propto \exp[\,-\,(\zeta^2)/2s_1]$

$$z_2 = x + \zeta_2 \qquad \zeta_2 = \mathcal{N}[0, s_2]$$

density function $p_2(\zeta) \propto \exp[\,-\,(\zeta^2)/2s_2]$

- ζ_1 and ζ_2 mutually independent

What is the conditional probability $P(x = \xi \mid z_1, z_2)$ that x be equal to some value ξ ?

$z_1 = x + \zeta_1$ density function $p_1(\zeta) \propto \exp[-(\zeta^2)/2s_1]$

$z_2 = x + \zeta_2$ density function $p_2(\zeta) \propto \exp[-(\zeta^2)/2s_2]$

ζ_1 and ζ_2 mutually independent

$x = \xi \Leftrightarrow \zeta_1 = z_1 - \xi$ and $\zeta_2 = z_2 - \xi$

- $P(x = \xi \mid z_1, z_2) \propto p_1(z_1 - \xi)\, p_2(z_2 - \xi)$

$$\propto \exp[-(\xi - x^a)^2/2p^a]$$

where $1/p^a = 1/s_1 + 1/s_2$, $x^a = p^a (z_1/s_1 + z_2/s_2)$

Conditional probability distribution of x, given z_1 and z_2 : $\mathcal{N}[x^a, p^a]$

$p^a < (s_1, s_2)$ independent of z_1 and z_2

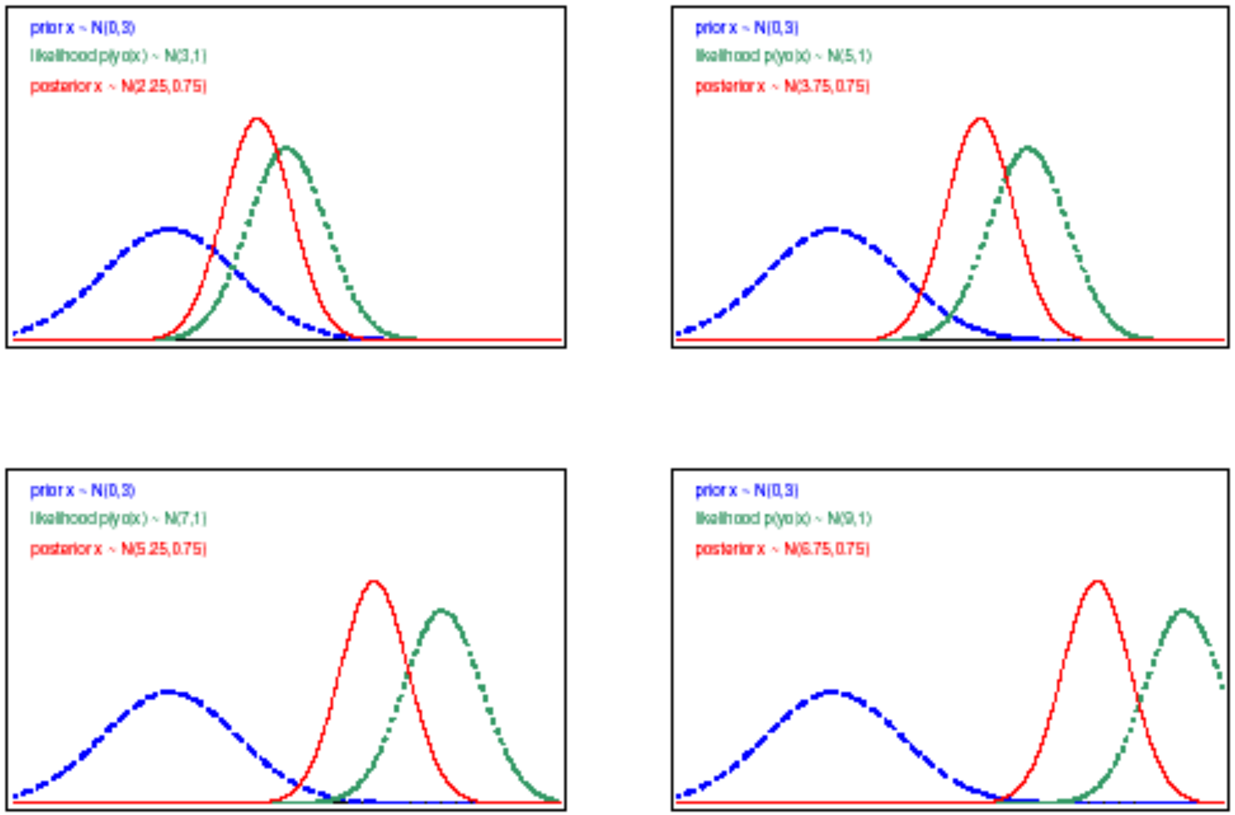


Fig. 1.1: Prior pdf $p(x)$ (dashed line), posterior pdf $p(x|y^o)$ (solid line), and Gaussian likelihood of observation $p(y^o|x)$ (dotted line), plotted against x for various values of y^o. (Adapted from Lorenc and Hammon 1988.)

Conditional expectation x^a minimizes following scalar *objective function*, defined on ξ-space

$$\xi \rightarrow \mathcal{J}(\xi) \equiv (1/2)\,[(z_1 - \xi)^2 / s_1 + (z_2 - \xi)^2 / s_2\,]$$

In addition

$$p^a = 1/\,\mathcal{J}''(x^a)$$

Conditional probability distribution in Gaussian case

$$P(x = \xi \mid z_1, z_2) \propto \exp[\,-\underbrace{(\xi - x^a)^2/2p^a}_{\mathcal{J}(\xi)\,+\,Cst}]$$

Estimate

$$x^a = p^a \,(z_1/s_1 + z_2/s_2)$$

with error p^a such that

$$1/p^a = 1/s_1 + 1/s_2$$

can also be obtained, independently of any Gaussian hypothesis, as simply corresponding to the linear combination of z_1 and z_2 that minimizes the error $E\,[(x^a{-}x)^{\,2}]$

Best Linear Unbiased Estimator (BLUE)

Bayesian estimation

State vector x, belonging to *state space* $\mathcal{S}$ ($\dim \mathcal{S} = n$), to be estimated.

Data vector z, belonging to *data space* $\mathcal{D}$ ($\dim \mathcal{D} = m$), available.

$$z = F(x, \zeta) \qquad (1)$$

where ζ is a random element representing the uncertainty on the data (or, more precisely, on the link between the data and the unknown state vector).

For example

$$z = \Gamma x + \zeta$$

Bayesian estimation (continued)

Probability that $x = \xi$ for given ξ ?

$$x = \xi \quad \Rightarrow \quad z = F(\xi, \zeta)$$

$$P(x = \xi \mid z) = P[z = F(\xi, \zeta)] \,/\, \int_{\xi'} P[z = F(\xi', \zeta)]$$

Unambiguously defined iff, for any ζ, there is at most one x such that (1) is verified.

$\Leftrightarrow$ data contain information, either directly or indirectly, on any component of x. *Determinacy* condition.

Bayesian estimation is however impossible in its general theoretical form in meteorological or oceanographical practice because

- It is impossible to explicitly describe a probability distribution in a space with dimension even as low as $n \approx 10^3$, not to speak of the dimension $n \approx 10^{6\text{-}9}$ of present Numerical Weather Prediction models (the *curse of dimensionality)*.

- Probability distribution of errors on data very poorly known (model errors in particular).

One has to restrict oneself to a much more modest goal. Two approaches exist at present

- Obtain some 'central' estimate of the conditional probability distribution (expectation, mode, …), plus some estimate of the corresponding spread (standard deviations and a number of correlations).

- Produce an ensemble of estimates which are meant to sample the conditional probability distribution (dimension $N \approx O(10\text{-}100)$).

Random vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T = (x_i)$ (*e. g.* pressure, temperature, abundance of given chemical compound at n grid-points of a numerical model)

- Expectation $E(\boldsymbol{x}) \equiv [E(x_i)]$; centred vector $\boldsymbol{x}' \equiv \boldsymbol{x} - E(\boldsymbol{x})$

- Covariance matrix

$$E(\boldsymbol{x}'\boldsymbol{x}'^T) = [E(x_i' x_j')]$$

dimension nxn, symmetric non-negative (strictly definite positive except if linear relationship holds between the x_i'‘s with probability 1).

- Two random vectors

$\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$

$\boldsymbol{y} = (y_1, y_2, \ldots, y_p)^T$

$$E(\boldsymbol{x}'\boldsymbol{y}'^T) = E(x_i' y_j')$$

dimension nxp

Covariance matrices will be denoted

$$C_{\boldsymbol{xx}} \equiv E(\boldsymbol{x}'\boldsymbol{x}'^{\mathrm{T}})$$

$$C_{\boldsymbol{xy}} \equiv E(\boldsymbol{x}'\boldsymbol{y}'^{\mathrm{T}})$$

Random function $\Phi(\xi)$ (field of pressure, temperature, abundance of given chemical compound, … ; ξ is now spatial and/or temporal coordinate)

- Expectation $E[\Phi(\xi)]$; $\Phi'(\xi) \equiv \Phi(\xi) - E[\Phi(\xi)]$
- Variance $Var[\Phi(\xi)] = E\{[\Phi'(\xi)]^2\}$

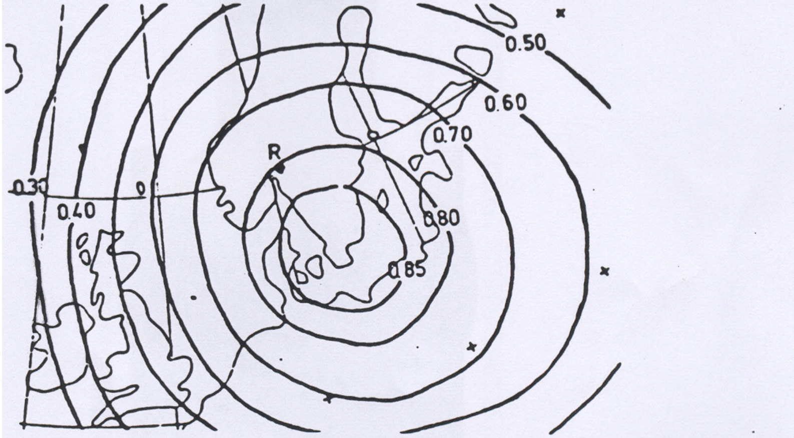
- Covariance function

$$(\xi_1, \xi_2) \rightarrow C_{\Phi}(\xi_1, \xi_2) \equiv E[\Phi'(\xi_1)\, \Phi'(\xi_2)]$$

- Correlation function

$$Cor_{\Phi}(\xi_1, \xi_2) \equiv E[\Phi'(\xi_1)\, \Phi'(\xi_2)] \,/\, \{Var[\Phi(\xi_1)]\, Var[\Phi(\xi_2)]\}^{1/2}$$

.: Isolines for the auto-correlations of the 500 mb geopotential between the station in Hannover and surrounding stations.
From Bertoni and Lund (1963)



: Isolines of the cross-correlation between the 500 mb geopotential in station 01 384 (R) and the surface pressure in surrounding stations.

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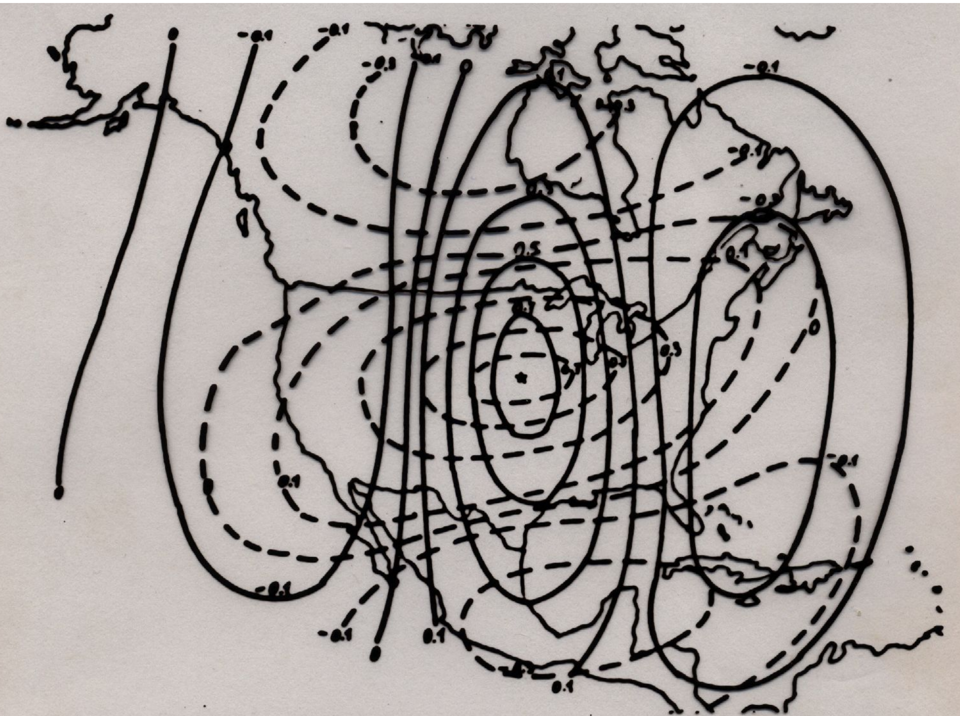

Figure 4.2.4.3: Isolines for the auto-correlation of the 500 mb u-wind component (dashed line) and the auto-correlation of the 500 mb v-wind component (full line). The "star" indicates the position of the reference station. (From Buel (1972).

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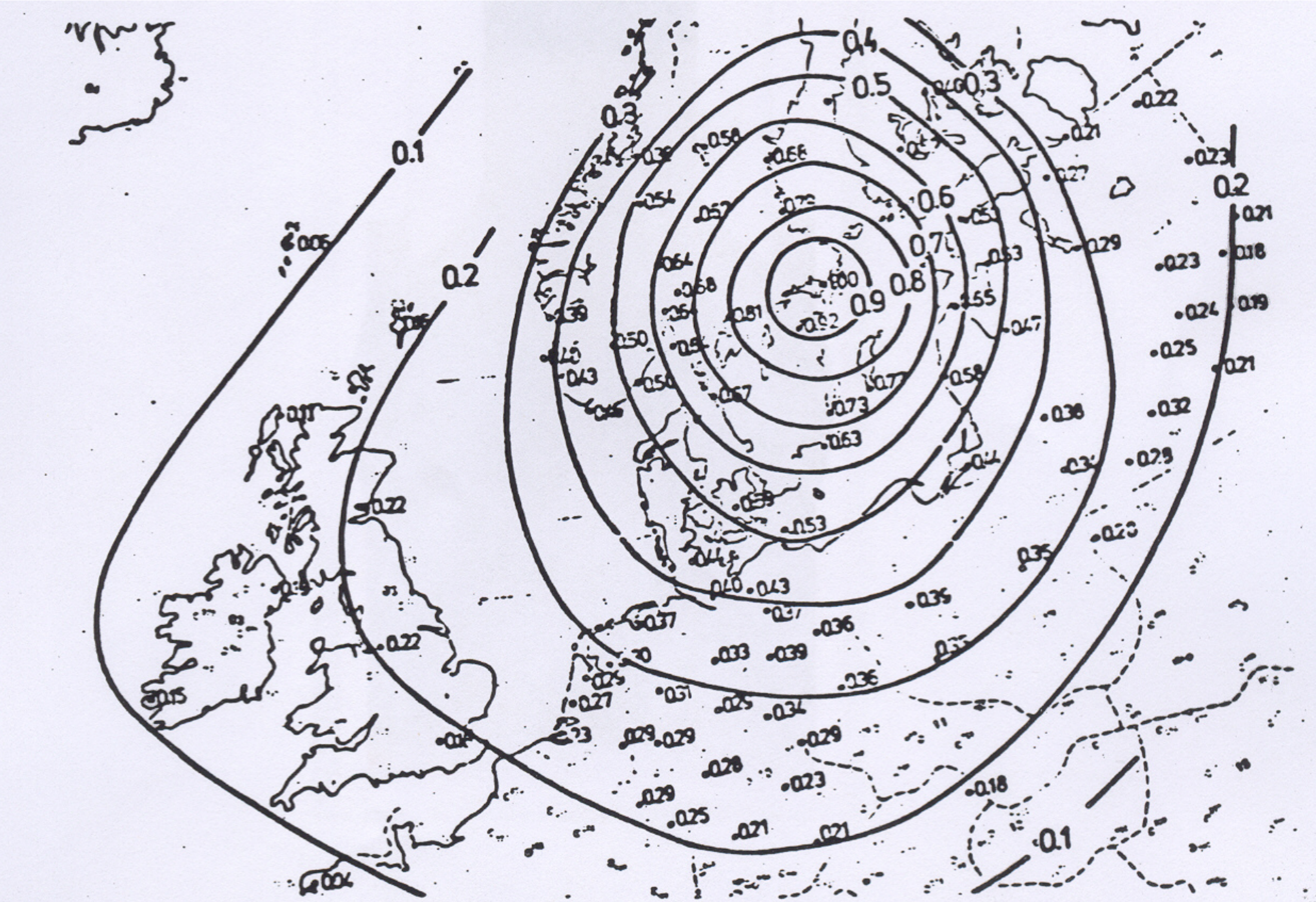

Figure 5.1.1.4.1 Auto-correlation of errors in 12h numerical forecasts of surface pressure in a reference station (Stockholm) and other stations.

After N. Gustafsson

Optimal Interpolation

Random field $\Phi(\xi)$

Observation network $\xi_1, \xi_2, \ldots, \xi_p$

For one particular realization of the field, observations

$y_j = \Phi(\xi_j) + \varepsilon_j \quad , \; j = 1, \ldots, p \qquad ,$ making up vector $\boldsymbol{y} = (y_j)$

Estimate $x = \Phi(\xi)$ at given point ξ, in the form

$$x^a = \alpha + \Sigma_j \, \beta_j \, y_j \; = \alpha + \boldsymbol{\beta}^T \boldsymbol{y} \qquad , \qquad \text{where } \boldsymbol{\beta} = (\beta_j)$$

α and the β_j's being determined so as to minimize the expected quadratic estimation error $E[(x\text{-}x^a)^2]$

Optimal Interpolation (continued 1)

Solution

$$x^a = E(x) + E(x'\mathbf{y}'^T)\,[E(\mathbf{y}'\mathbf{y}'^T)]^{-1}\,[\mathbf{y} - E(\mathbf{y})]$$
$$= E(x) + \boldsymbol{C}_{x\mathbf{y}}\,[\boldsymbol{C}_{\mathbf{yy}}]^{-1}\,[\mathbf{y} - E(\mathbf{y})]$$

i.e.,
$$\boldsymbol{\beta}^T = C_{x\mathbf{y}}\,[C_{\mathbf{yy}}]^{-1}$$
$$\alpha = E(x) - \boldsymbol{\beta}^T E(\mathbf{y})$$

Estimate is unbiased $E(x-x^a) = 0$

Minimized quadratic estimation error

$$E[(x-x^a)^2] = E(x'^2) - E[(x'^a)^2])$$
$$= \boldsymbol{C}_{xx} - \boldsymbol{C}_{x\mathbf{y}}\,[\boldsymbol{C}_{\mathbf{yy}}]^{-1}\,\boldsymbol{C}_{\mathbf{y}x}$$

Estimation made in terms of deviations x' and $\mathbf{y}'$ from expectations $E(x)$ and $E(\mathbf{y})$.

Optimal Interpolation (continued 2)

$$x^a = E(x) + E(x'\mathbf{y}'^{\mathrm{T}})\,[E(\mathbf{y}'\mathbf{y}'^{\mathrm{T}})]^{-1}\,[\mathbf{y} - E(\mathbf{y})]$$

$$y_j = \Phi(\xi_j) + \varepsilon_j$$

$$E(y_j'y_k') = E[\Phi'(\xi_j) + \varepsilon_j'][\Phi'(\xi_k) + \varepsilon_k']$$

If observation errors ε_j are mutually uncorrelated, have common variance r, and are uncorrelated with field Φ, then

$$E(y_j'y_k') = C_\Phi(\xi_j, \xi_k) + r\delta_{jk}$$

and

$$E(x'y_j') = C_\Phi(\xi, \xi_j)$$

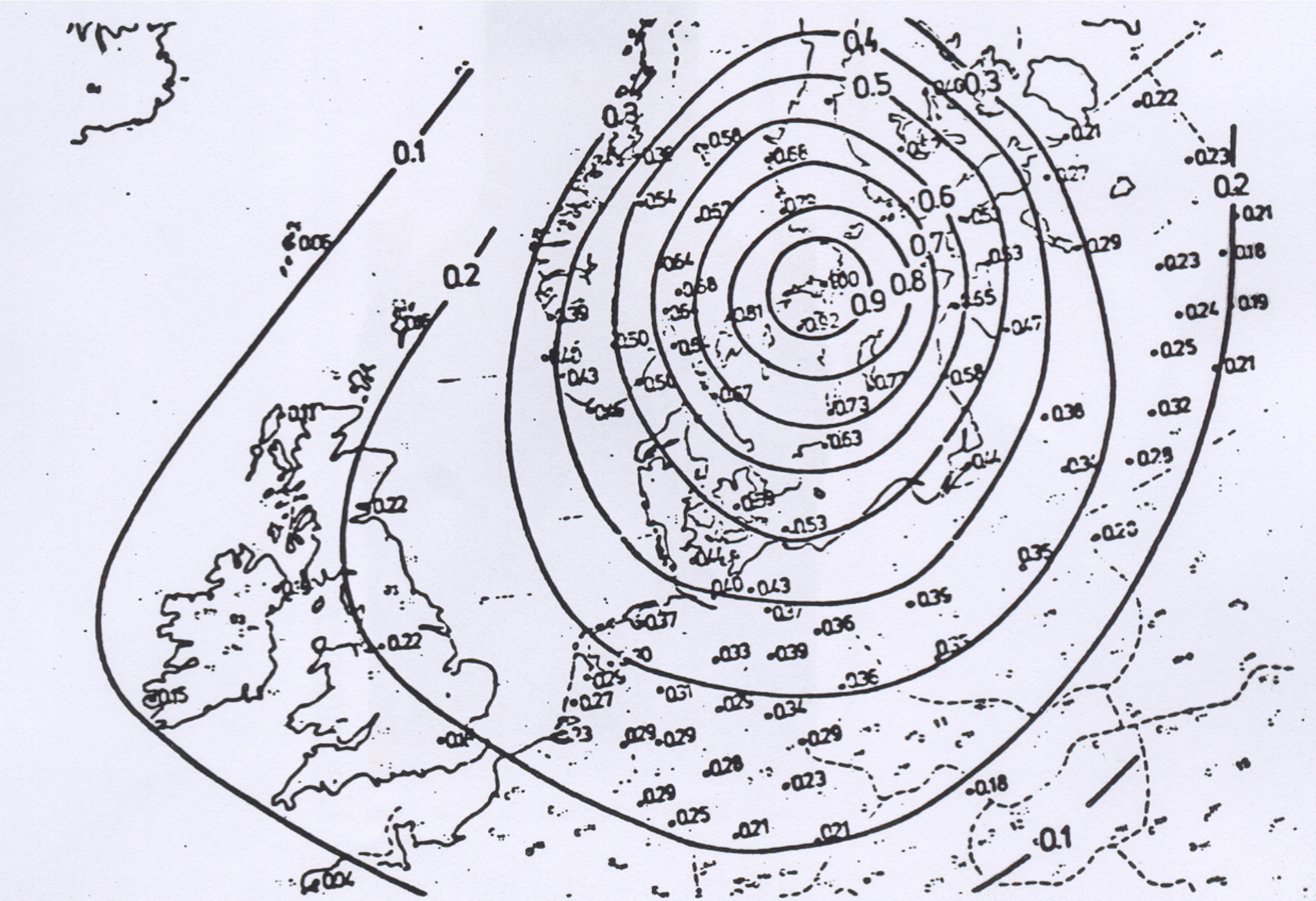

Figure 5.1.1.4.1 Auto-correlation of errors in 12h numerical forecasts of surface pressure in a reference station (Stockholm) and other stations.

After N. Gustafsson

Cours à venir

~~Jeudi 19 avril~~

~~Jeudi 26 avril~~

~~Jeudi 3 mai~~

Lundi 14 mai

Jeudi 17 mai

Jeudi 24 mai

Jeudi 7 juin

Jeudi 14 juin

De 10h00 à 12h30, Salle E314, 3ième étage, Département de Géosciences, École Normale Supérieure, 24, rue Lhomond, Paris 5