

Localized/Shrinkage Kriging Predictors

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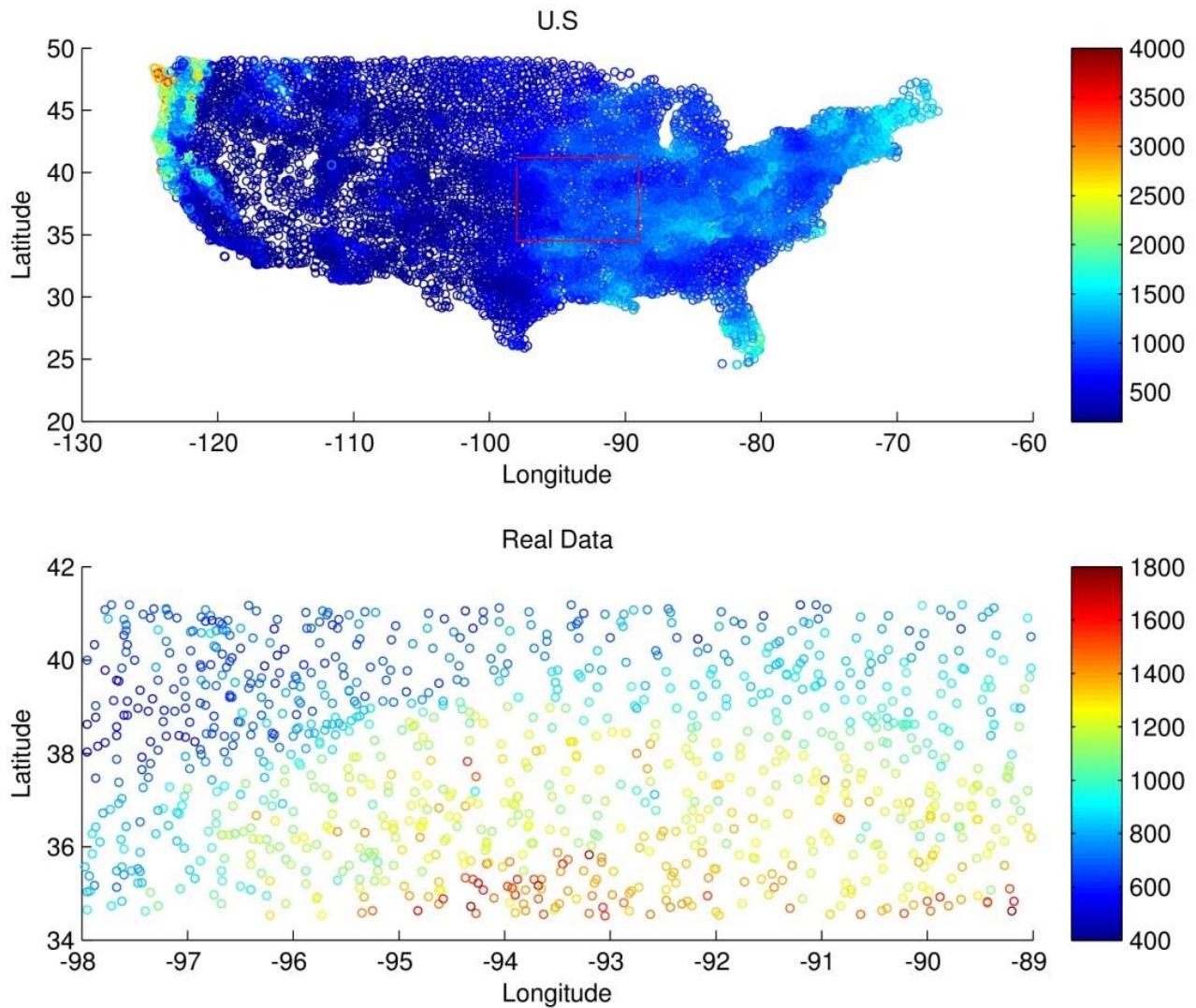
Gløshaugen March 2021

Zeytu & Omre (2016) - Math Geosc
Røislien & Omre (2006) – Math Geosc
Efron & Morris (1973) – JASA
+ Charles Stein – of course !

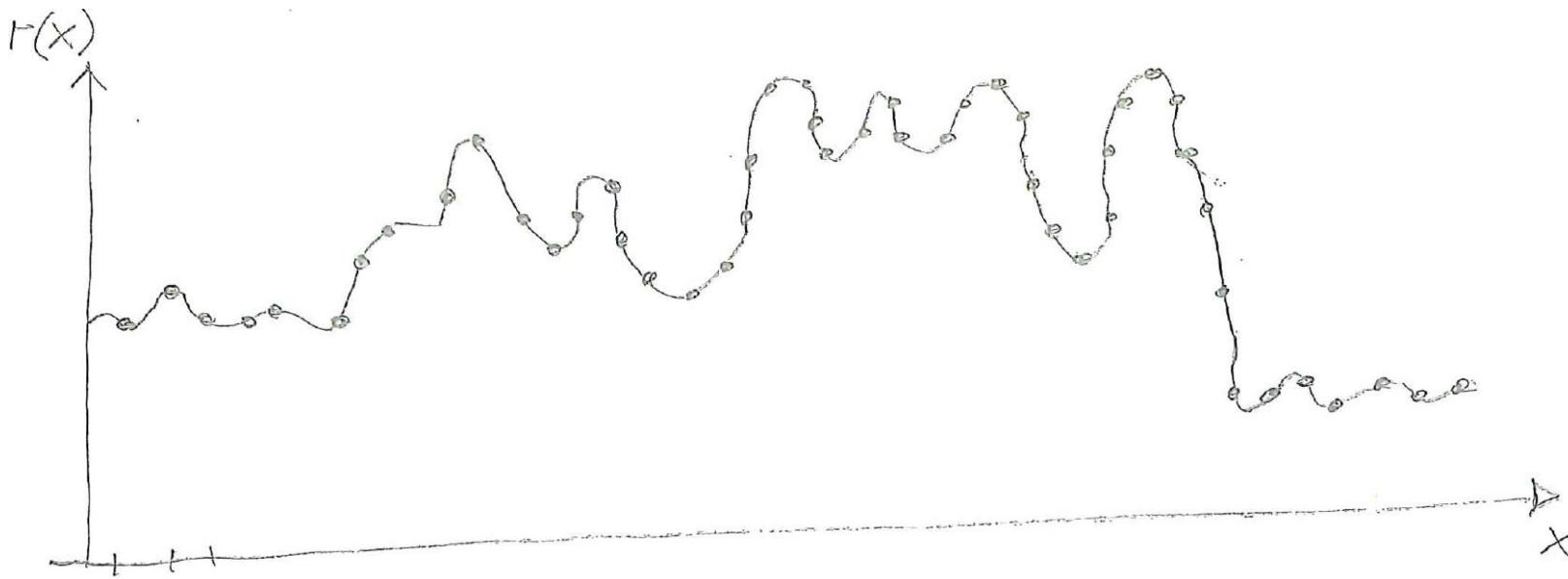
Data Set

Precipitation in 1997
- spatial problem only

Subset n=1001



Data Acquisition



Likelihood - Dirac-linear

$$\left[\pi_0 | \{r(x); x \in \mathcal{D}\} \right] = H(r(x); x \in \mathcal{D}) = \begin{bmatrix} r(x_1) \\ \vdots \\ r(x_n) \end{bmatrix} + \cancel{\times} = \begin{bmatrix} r_1 \\ \vdots \\ r_n \end{bmatrix}$$

TRAD KRIEING

Prior = GaussRF (μ, σ^2, θ)

$$\{r(x) = \mu + \cancel{\sum_{\ell} \mu_{\ell} g_{\ell}(x)} + \sigma r_s(x)\} \stackrel{\uparrow}{\sim} \text{GaussRF}(0, 1, \theta)$$

$$E\{r(x)\} = \mu$$

$$\text{Cov}\{r(x'), r(x'')\} = \sigma^2 \rho(\tau; \theta) \longrightarrow \exp\left\{-\frac{[z]}{[z_0]}\right\}$$

$$\downarrow \\ \omega_0, \beta_0$$

Predictor $r(x_t) = r_t$

$$\begin{aligned}\hat{r}_{+10} &= \hat{\mu}_{+10} = \mu + \sigma^2 \omega_{+0}^T [\sigma^2 R_{00}]^{-1} [r_0 - \mu \vec{w}_n] \\ &= \mu + \omega_{+0}^T R_{00}^{-1} [r_0 - \mu \vec{w}_n] - \text{indep } \sigma^2\end{aligned}$$

$$\begin{aligned}\hat{\sigma}_{+10}^2 &= \sigma^2 - \sigma^2 \omega_{+0}^T [\sigma^2 R_{00}]^{-1} \sigma^2 \omega_{+0} \\ &= \sigma^2 \left[1 - \omega_{+0}^T R_{00}^{-1} \omega_{+0} \right] - \text{indep } \frac{r_0}{\mu}\end{aligned}$$

→ Localization:

$$\begin{array}{ccc} & \text{binary} & \\ & \text{selection} & \\ & \text{matrix} & \\ R_0 & \xrightarrow{\quad \quad \quad \quad \quad} & \omega_{+0}^t = G_{+}^{n_{+}} \omega_{+0} \\ n \times 1 & n_{+} \times 1 & n_{+} \times 1 \\ R_0^+ = G_{+}^{n_{+}} R_0 & & \\ & & \\ & \xrightarrow{n_{+} \times 1} & \mathcal{S}_{00}^t = G_{+}^{n_{+}} \mathcal{S}_{00} G_{+}^{n_{+} T} \\ & & \end{array}$$

Good approx!

Model parameters: $\left\{ \begin{array}{l} \mu \in \mathbb{R} \\ \sigma^2 \in \mathbb{R}_+ \\ \theta \rightarrow \exp\left\{ \frac{\beta z}{z_0} \right\} \end{array} \right.$

Parameter inference

[vel_{o,2}]

Assume known: $\rho(\varepsilon) = \exp\left\{-\frac{|\varepsilon|^\nu}{\varepsilon_0}\right\} \rightarrow \mathcal{R}_{oo}$
ML estimators:

n × n

$$\hat{\mu} = [\mathbf{i}_n^T \Omega_{oo}^{-1} \mathbf{i}_n]^{-1} [\mathbf{i}_n^T \Omega_{oo}^{-1} \mathbf{r}_o],$$

$$\hat{\sigma}^2 = \frac{1}{n} [\mathbf{r}_o - \hat{\mu} \mathbf{i}_n]^T \Omega_{oo}^{-1} [\mathbf{r}_o - \hat{\mu} \mathbf{i}_n],$$

Localization more difficult!

GEN KRIEING

Prior - GaussRF $\left(\begin{bmatrix} \mu(x) \\ \sigma^2(x); x \in D \end{bmatrix}, \theta \right)$

$$\left\{ r(x) = \mu(x) + \cancel{\sum_{i=1}^n \rho_i g_i(x)} + \sigma(x) \zeta(x) \right\}$$

$$E\{ r(x) \} = \mu(x)$$

$$\text{Cov}\{ r(x'), r(x'') \} = \sigma(x') \sigma(x'') \rho(\tau; \theta)$$
$$\rightarrow \exp\left\{-\left[\frac{\tau}{\tau_0}\right]^2\right\}$$
$$\omega \xrightarrow{\downarrow} \mathcal{D}_{\omega_0}$$

Predictor: $\Gamma(x_+) = \Gamma_+$

$$\overset{1}{\Gamma}_{+10} = \mu_{+10} = \mu_+ + \sigma_+ \omega_{+0}^T \overset{\Gamma}{I}_0 \begin{bmatrix} \Gamma & S_0 & \Gamma \\ I_0 & S_0 & I_0 \\ 0 & 0 & 0 \end{bmatrix}^{-1} [\Gamma_0 - \mu_0] - \text{indep } \tilde{z}$$

$$\begin{bmatrix} \sigma_1 & & & \\ & \ddots & & 0 \\ 0 & & \ddots & \\ & & & \sigma_n \end{bmatrix}_{n \times n}$$

$$\begin{bmatrix} \mu_1 \\ \vdots \\ \mu_n \end{bmatrix}_{n \times 1}$$

$$\overset{2}{\sigma}_{+10}^2 = \sigma_+^2 - \sigma_+ \omega_{+0}^T \overset{\Gamma}{I}_0 \begin{bmatrix} \Gamma & S_0 & \Gamma \\ I_0 & S_0 & I_0 \\ 0 & 0 & 0 \end{bmatrix}^{-1} \overset{\Gamma}{I}_0 \omega_{+0} - \text{indep } \frac{\Gamma_0}{\mu_0}$$

Localization:

↑ Good approx

Model parameters: $\mu_0 \in \mathbb{R}^n$

$\Gamma_0 \in \mathbb{R}^n$

$\Theta \rightarrow \exp\left\{-\frac{1}{\varepsilon_0} T^\mu\right\}$

$\mu_T \in \mathbb{R}$

$\sigma_T^2 \in \mathbb{R}_+$

Synthetic Example

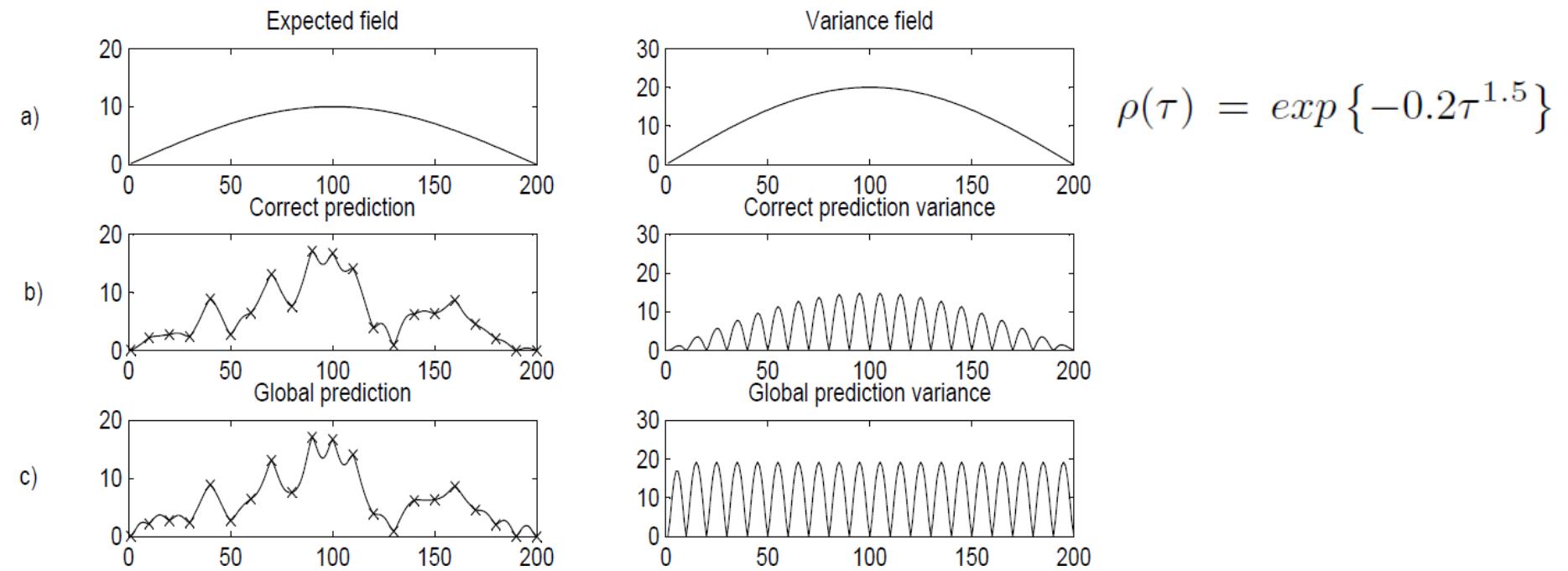


Fig. 10 General Gaussian random field. Expectation and variance field (a), Predictions and prediction variances for one realization (b-e)

Parameter inference

Assume known: $\rho(\tau) = \exp\left\{-\frac{[\tau]}{\tau_0}\right\} \rightarrow \mathcal{R}_{oo}$
 $n \times n$

Focus on location $x_* \rightarrow \mathcal{D}_o^k \subset \mathcal{D}; r_o^* = G_o^k r_o$

$k \times 1 \quad k \times n \quad n \times 1$

→ Inference model in $\mathcal{D}_o^k \subset \mathcal{D}$:

$$\text{GaussRF}(\mu_o, \sigma_o^2) \rightarrow \begin{matrix} \mu_o \\ \sigma_o^2 \end{matrix}$$

$$\hat{\mu} = [\mathbf{i}_n^T \Omega_{oo}^{-1} \mathbf{i}_n]^{-1} [\mathbf{i}_n^T \Omega_{oo}^{-1} \mathbf{r}_o],$$

$$\hat{\sigma}^2 = \frac{1}{n} [\mathbf{r}_o - \hat{\mu} \mathbf{i}_n]^T \Omega_{oo}^{-1} [\mathbf{r}_o - \hat{\mu} \mathbf{i}_n],$$

Challenge: Bias/Variance
Trade-off

Synthetic Example

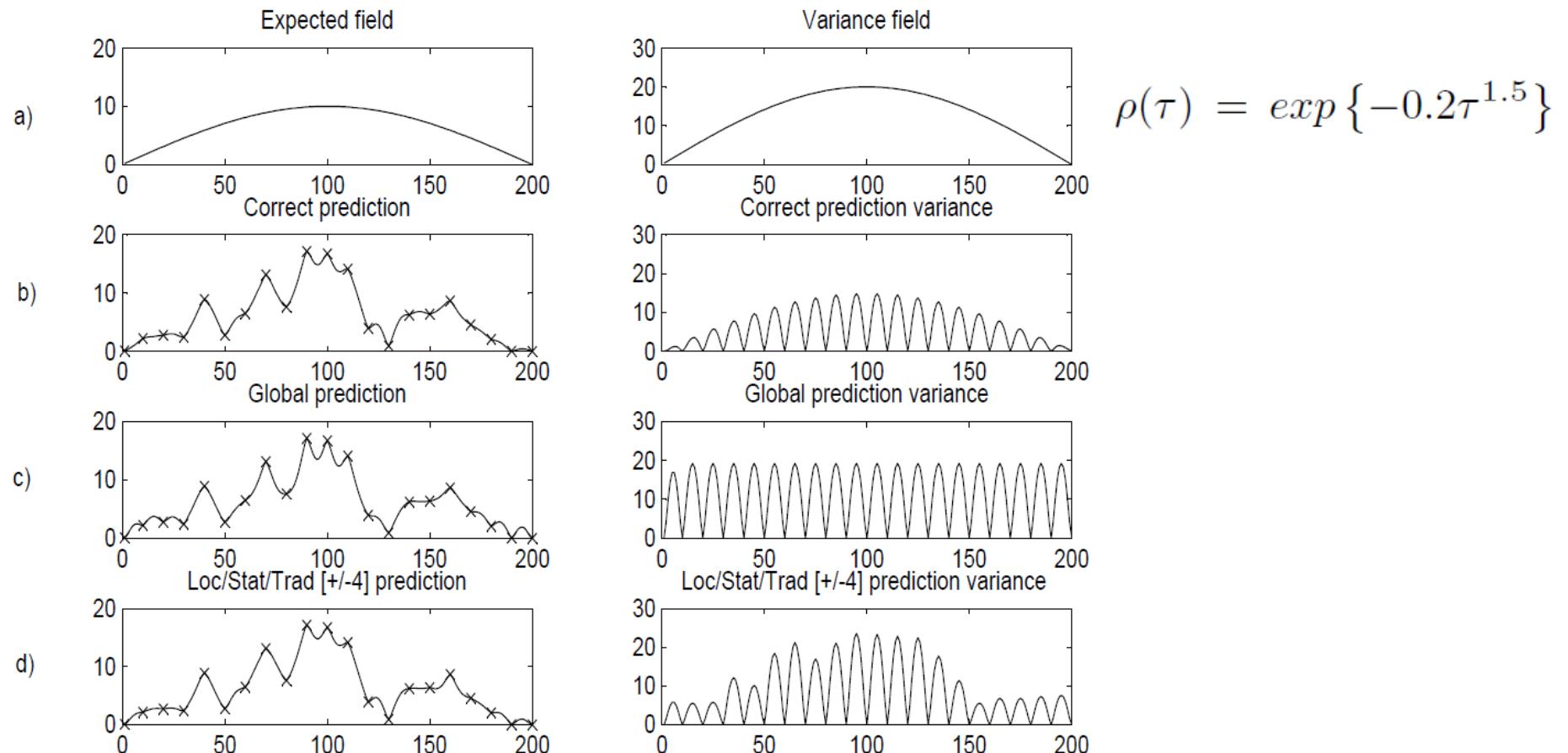


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Bayesian Inference

Inference model in $\mathcal{D}_o^k \subset \mathcal{D}_i$; $R_o^k = G_o K_o$

$$T\text{-RF}(\mu_m, \tau_m, \xi_s, \gamma_s)$$

Røislien & Omre (2006)

Defined by:

$$[r(x) | m, s^2] \rightarrow \text{GaussRF}(m, s^2)$$

Conjugate priors:

$$[m | s^2] \rightarrow \text{Gauss}(\mu_m, \tau_m s^2)$$

$$= [2\pi]^{\frac{-1}{2}} [\tau_m s^2]^{-\frac{1}{2}} \exp \left\{ \frac{-1}{2} [\tau_m s^2]^{-1} [m - \mu_m]^2 \right\}$$

$$s^2 \rightarrow \text{InvGam}(\xi_s, \gamma_s)$$

$$= [\Gamma(\xi_s)]^{-1} \gamma_s^{\xi_s} [s^2]^{-(\xi_s + 1)} \exp \left\{ -\gamma_s [s^2]^{-1} \right\}$$

Posterior E-estimators:

$$\hat{\mu}_o = \mu_{m|o} = E\{m|s^z, r_o^*\} =$$

$$\mu_{m|o} = \mu_m + \tau_m \mathbf{i}_n^T [\tau_m \mathbf{i}_n \mathbf{i}_n^T + \Omega_{oo}]^{-1} [\mathbf{r}_o - \mu_m \mathbf{i}_n]$$

$$\hat{\sigma}_o^2 = [z_{s|o} - 1] \hat{\sigma}_{s|o} = E\{s^z/r_o^*\} =$$

$$\xi_{s|o} = \xi_s + \frac{n}{2}$$

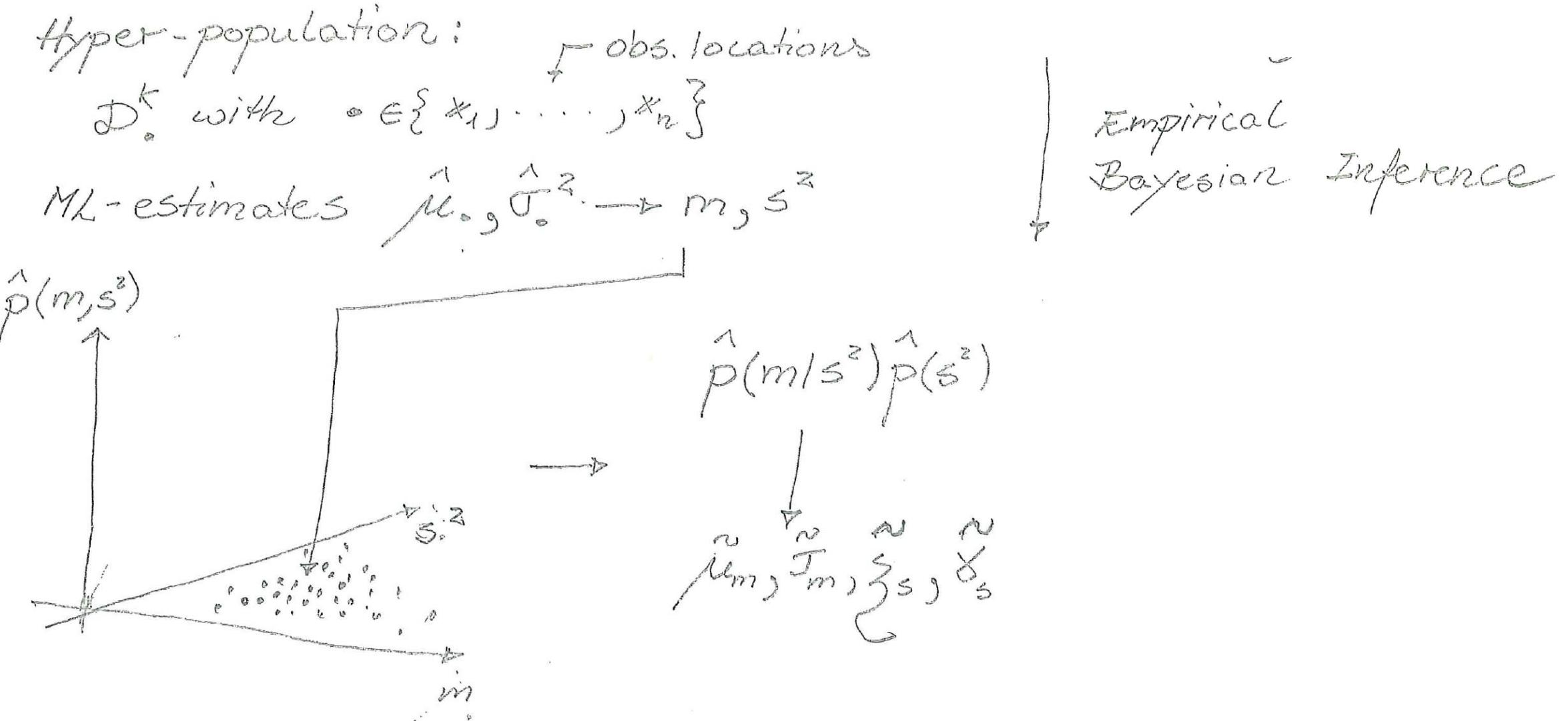
$$\gamma_{s|o} = \gamma_s + \frac{1}{2} \left[[\mathbf{r}_o - \mu_m \mathbf{i}_n]^T [\tau_m \mathbf{i}_n \mathbf{i}_n^T + \Omega_{oo}]^{-1} [\mathbf{r}_o - \mu_m \mathbf{i}_n] \right]$$

Challenge: Elicitation of

$$, \mu_m, \tau_m, \xi_s, \delta_s$$

} Empirical
Bayesian Inference

→ Empirical Bayes elicitation
Efron & Morris (1973)



localized Predictors

Challenge: No global anchoring?

NOTE:
Cross-validation (CV) undercorrect model.

$$e_i = \left[\frac{r_i - \hat{r}_{i|O-i}}{\hat{\sigma}_{i|O-i}} \right] \rightsquigarrow \text{Gauss}(0, 1)$$

In Practice use:

CV-corrected (cvc) Predictor:

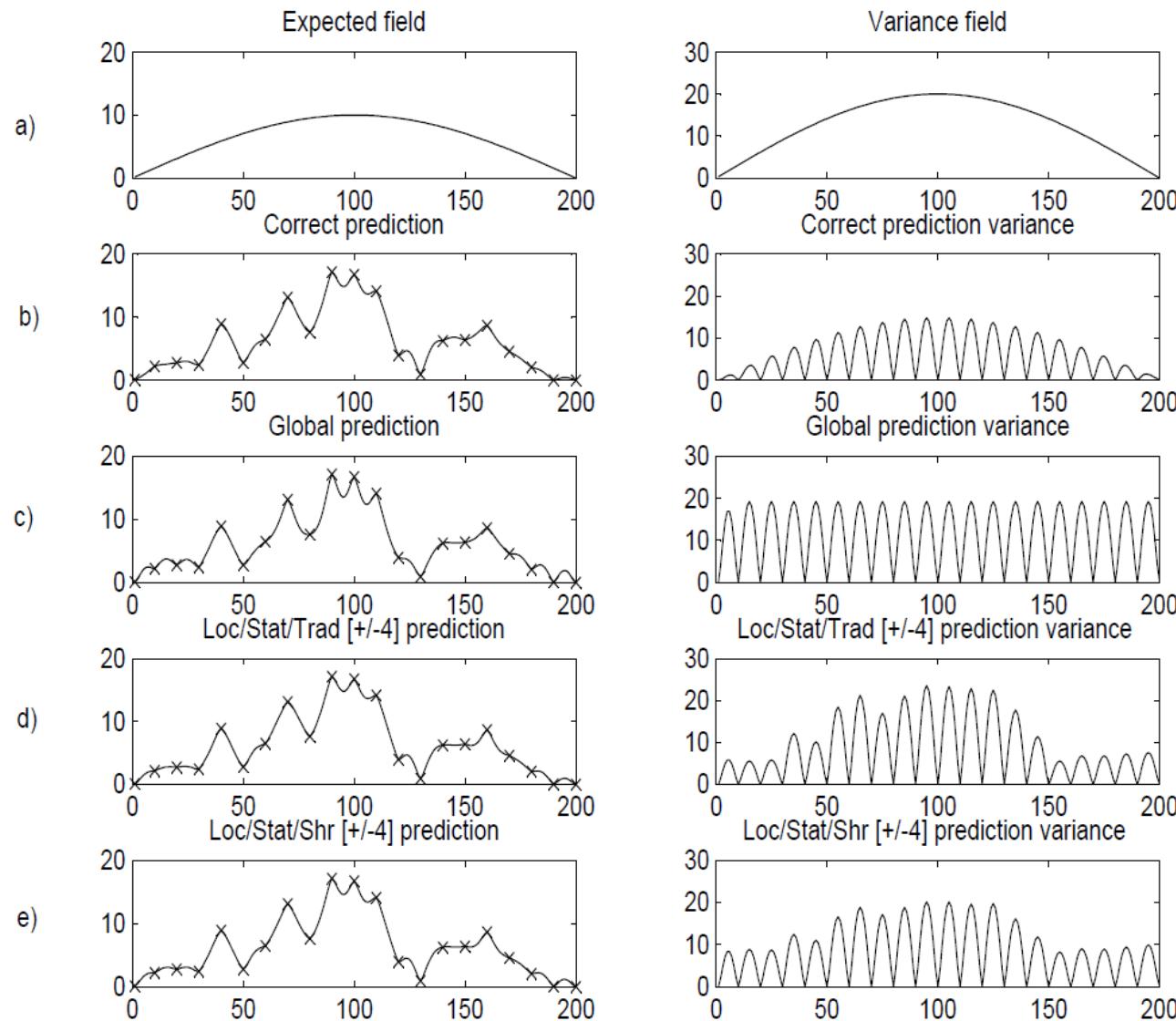
$$\hat{r}_{i|O} = \hat{r}_{i|O} + \hat{\sigma}_{i|O} / \mu_e$$

$$\hat{\sigma}_{i|O}^2 = \sum_i \hat{e}_i^2 \hat{\sigma}_{i|O}^2$$

NOTE:

Use CV as criterion

Synthetic Example



$$\rho(\tau) = \exp \{-0.2\tau^{1.5}\}$$

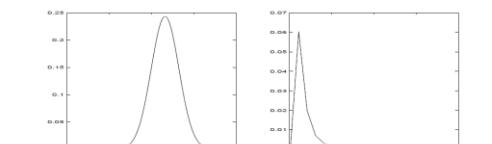
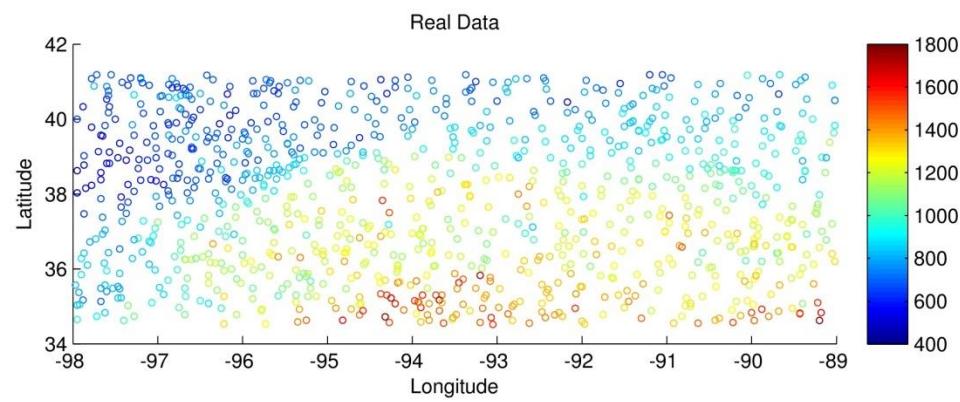
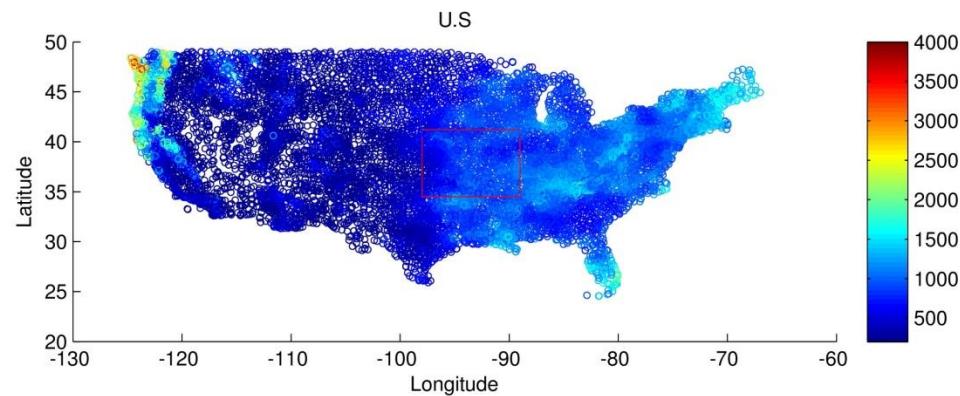


Fig. 11 General Gaussian random field. Prior model for expectation and variance for one realization

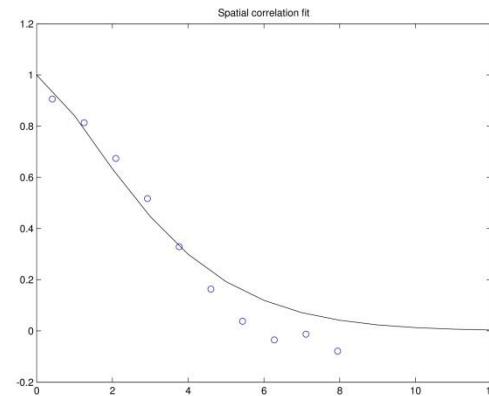
Fig. 10 General Gaussian random field. Expectation and variance field (a), Predictions and prediction variances for one realization (b-e)

Evaluation Data - US Precipitation 1997 – subset n=1001

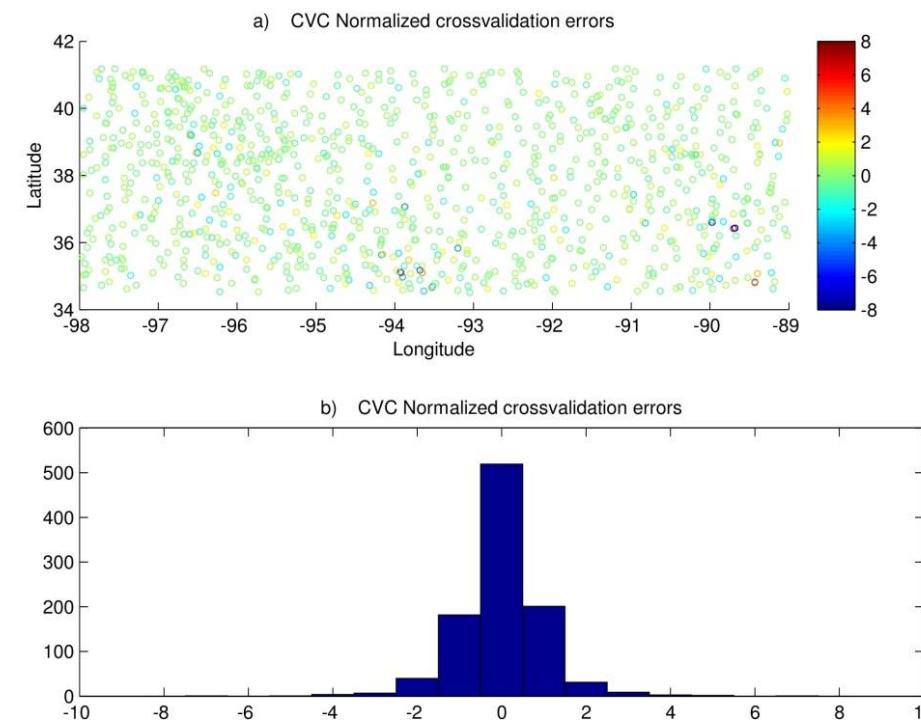
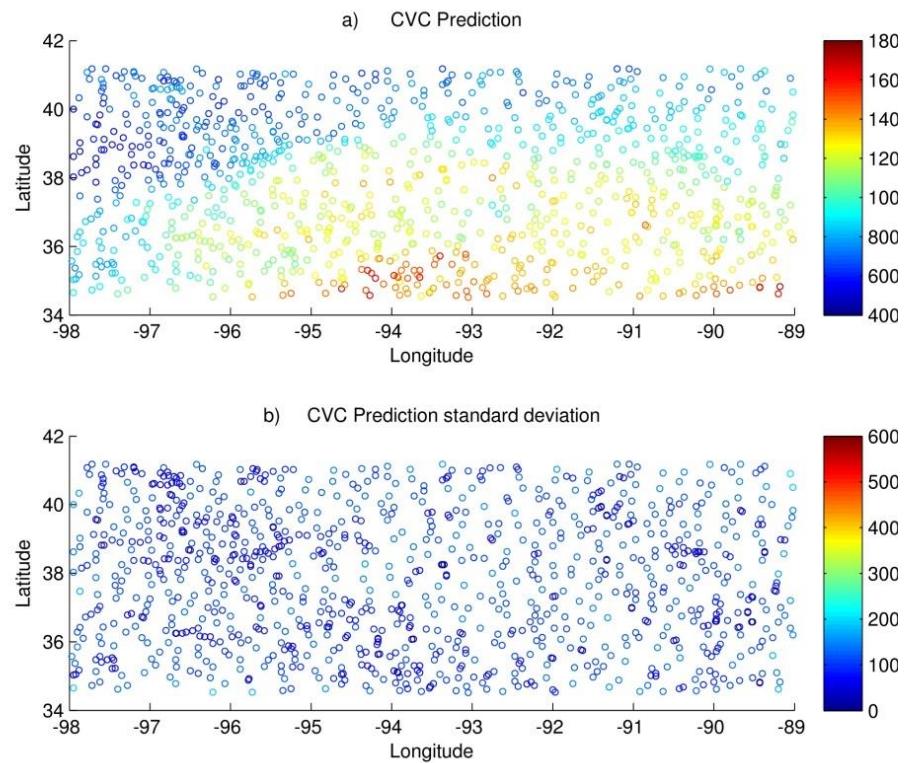


Estimated global spatial correlation function:

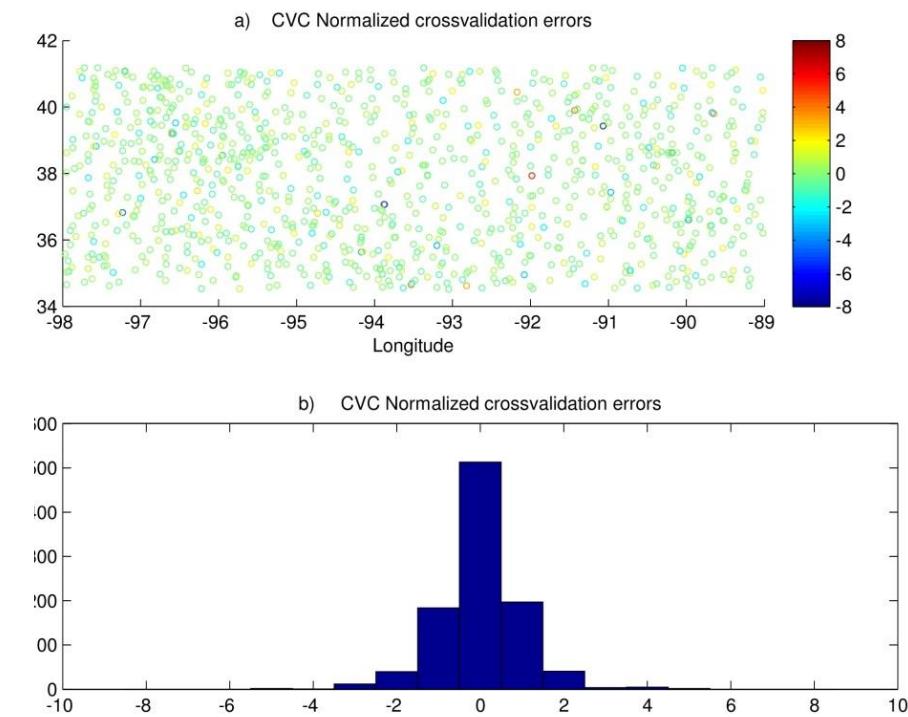
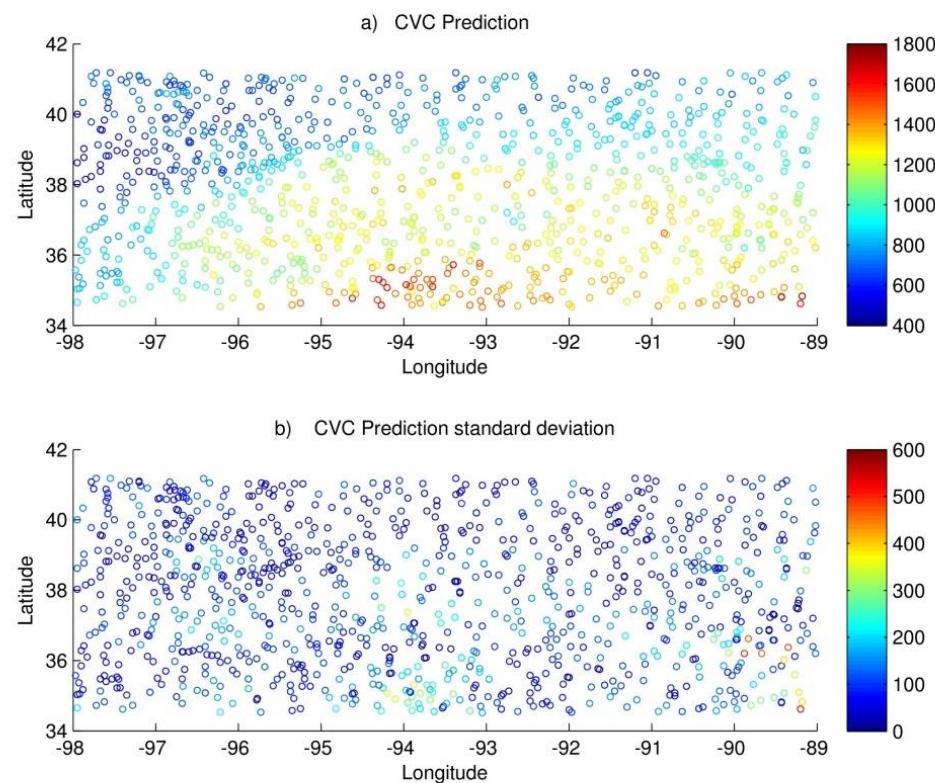
$$\text{Corr}\{r(x'), r(x'')\} = \rho(x' - x'')$$



Glob/Stat/Trad k=1000 CVC Kriging Predictor:



Loc/Stat/Trad k=10 CVC Kriging Predictor:



Loc/Stat/Shr k=10 CVC Kriging Predictor:

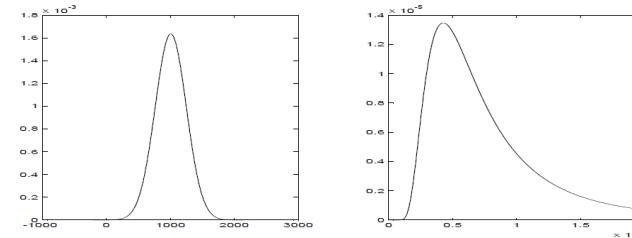
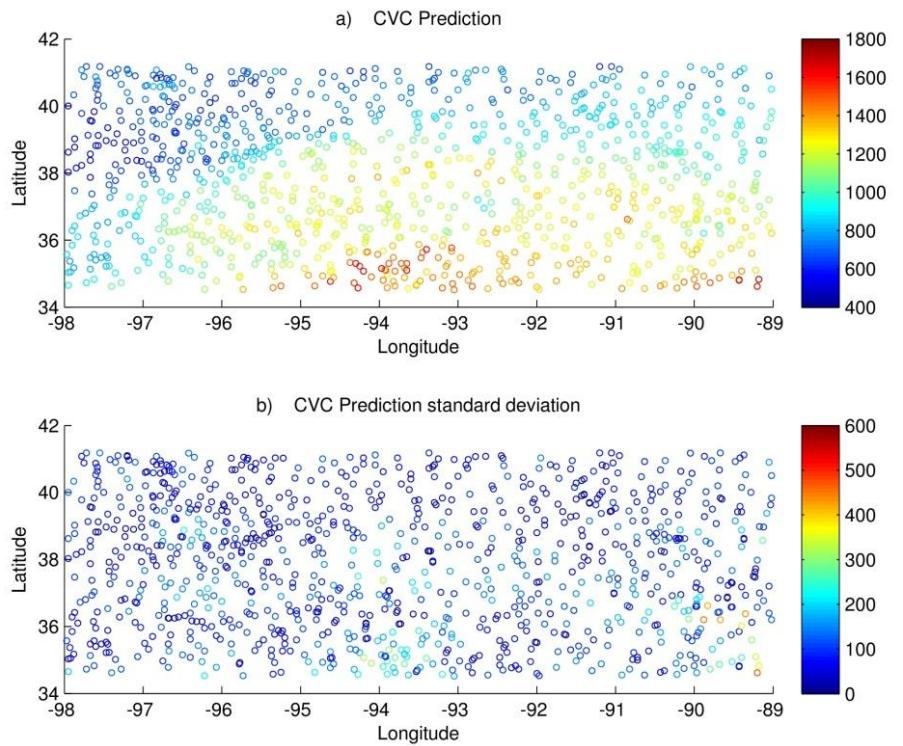
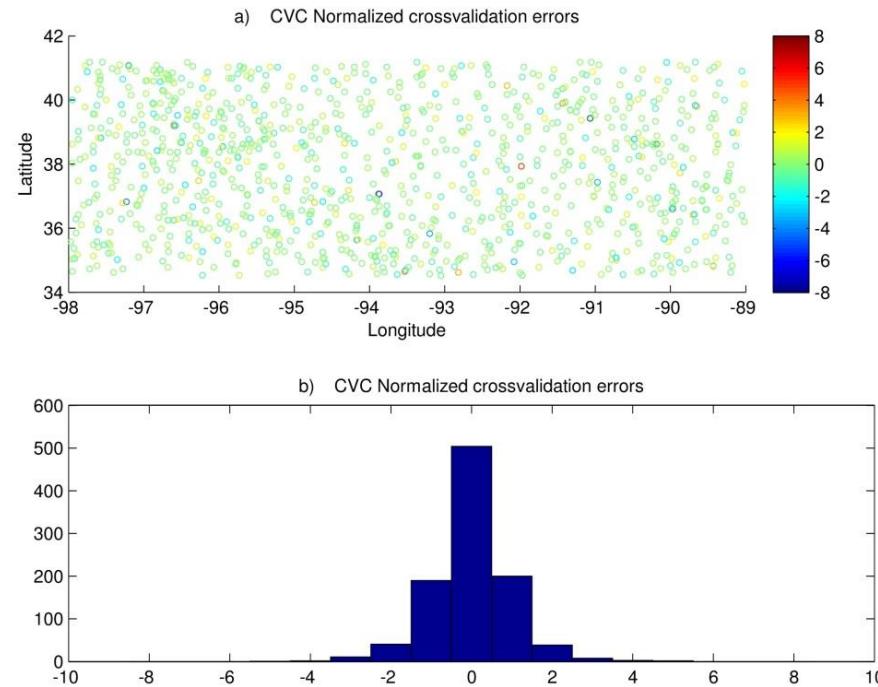


Fig. 9 US Precipitation study. Priors model for expectation and variance



Empirical Evaluation

Empirical study – Summary Table:

Based on CV:

$$PMSE = \frac{1}{n} \sum_{i=1}^n \left[r_i - \hat{r}_{i|0-i} \right]^2 - \text{prediction accuracy}$$

$$VMSE = \frac{1}{n} \sum_{i=1}^n \left[\frac{\left[r_i - \hat{r}_{i|0-i} \right]^2}{\hat{s}_{i|0-i}^2} - 1 \right]^2 - \text{variance accuracy}$$

Table 1 US Precipitation study. Evaluation criteria: Mean normalized error (MNE), Mean square normalized error (MSNE), Prediction mean squared error (PMSE) and Variance mean squared error (VMSE)

Model	Localized/Stationary			Localized/Non-stationary	
	Traditional		Shrinkage	Traditional	Shrinkage
Test D.	$k = 1,000$	$k = 10$	$k = 10$	$k = 10$	$k = 10$
MNE	1.0148e-17	-5.3792e-18	5.9892e-17	1.5084e-16	-1.1579e-16
MSNE	1.5399	2.9740	3.3928	9.2487	5.1702
PMSE	6.8758e + 03	6.8745e + 03	6.8654e + 03	2.2181e + 04	9.3555e + 03
VMSE	9.8749	5.9746	5.2027	4.0787	4.3475

Conclusion:

- Hierarchical non-stationary Gaussian RF – fully analytically tractable
- Localized model parameter inference – expectation & variance
- Robustified parameter inference by empirical Bayes approach
- Prediction by Localized/Shrinkage Kriging – analytically tractable
- Computer demands by Spatial Predictor is linear in no of observations.
- Spatial Prediction by ‘non-stationary spatial Covariance function’
- Encouraging results from empirical study – actually more than so !!!

EXTRA !

Kriging - Alternative views

Spatial variable $\{r(x); x \in D \subset \mathbb{R}^3\}$

Likelihood:

$$l(r) = f(r(x); x \in D) = \begin{bmatrix} r(x_1) \\ \vdots \\ r(x_n) \end{bmatrix} = \begin{bmatrix} t_1 \\ \vdots \\ t_n \end{bmatrix}$$

Prior - GaussRF($0, 1, \theta_0$) $\rightarrow \exp\left\{-\frac{z^2}{2\theta_0^2}\right\}$

$$E\{r(x)\} = 0$$

$$\text{Cov}\{r(x'), r(x'')\} = \exp\left\{-\frac{z^2}{2\theta_0^2}\right\} \rightarrow w_0, R_{00}$$

Prior - GaussRF($\theta_0, 1, \theta_0$) $\rightarrow \exp\left\{-\frac{\|x-x_0\|^2}{2\theta_0^2}\right\}$

$$E\{r(x)\} = 0$$

$$\text{Cov}\{r(x'), r(x'')\} = \exp\left\{-\frac{\|x'-x''\|^2}{2\theta_0^2}\right\} \rightarrow \omega_{0+} \mathcal{R}_{00}$$

Predictor $r(x_+) = \hat{r}_+$

$$\hat{r}_{+10} = \mu_{+10} = \omega_{+0}^T \mathcal{R}_{00}^{-1} r_0 \quad - \text{simple Kriging}$$

$1 \times n \quad n \times n \quad n \times 1$

$$\hat{\sigma}_{+10}^2 = \left[1 - \omega_{+0}^T \mathcal{R}_{00}^{-1} \omega_{+0} \right]$$

Closer look at Predictor

$$\hat{r}_{+0} = \alpha_{+0}^T \bar{\Sigma}_{00}^{-1} r_0 \quad - \text{simple Kriging}$$

Alt A-frod Kriging

$$= \underbrace{\alpha_{+0}^T}_{1 \times n} \cdot \underbrace{r_0}_{n \times 1} = \sum_{i=1}^n \alpha_i r_i$$

Lin in obs
 α_{+0} = dep x_+
dep $\rho(\cdot)$
dep x_0
indep r_0

Closer look at Predictor

$$\hat{r}_{+0} = \alpha_{+0}^T \beta_{00}^{-1} r_0 \quad - \text{simple Kriging}$$

A+B - dual Kriging

$$= \alpha_{+0}^T \cdot \beta_{+0} = \sum_{i=1}^n \beta_i \rho(x_+ - x_i) \text{ Lin in } \rho(\cdot),$$

β_{+0} - dep r_0
 α_{+0} - dep $\rho(\cdot)$
 x_0 - dep x_+
indep x_+

Note:

$$\left\{ \hat{r}(x) = \sum_{i=1}^n \beta_i \cdot \rho(x - x_i); x \in \mathcal{P} \right\} - \text{cont in } x \in \mathcal{P}$$

NOTE:

$$\left\{ \hat{f}(x) = \sum_{i=1}^n \beta_i \cdot \rho(x - x_i); x \in \mathcal{P} \right\} - \text{cont in } x \in \mathcal{P}$$

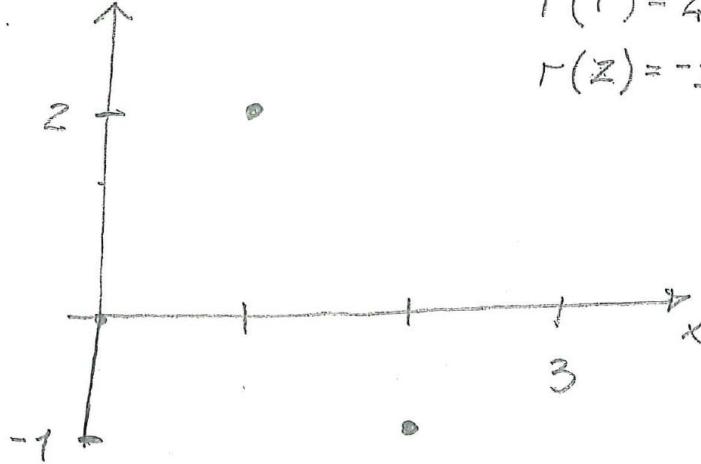
hence

$$\frac{d \hat{f}(x)}{dx} = \text{analytically tractable}$$

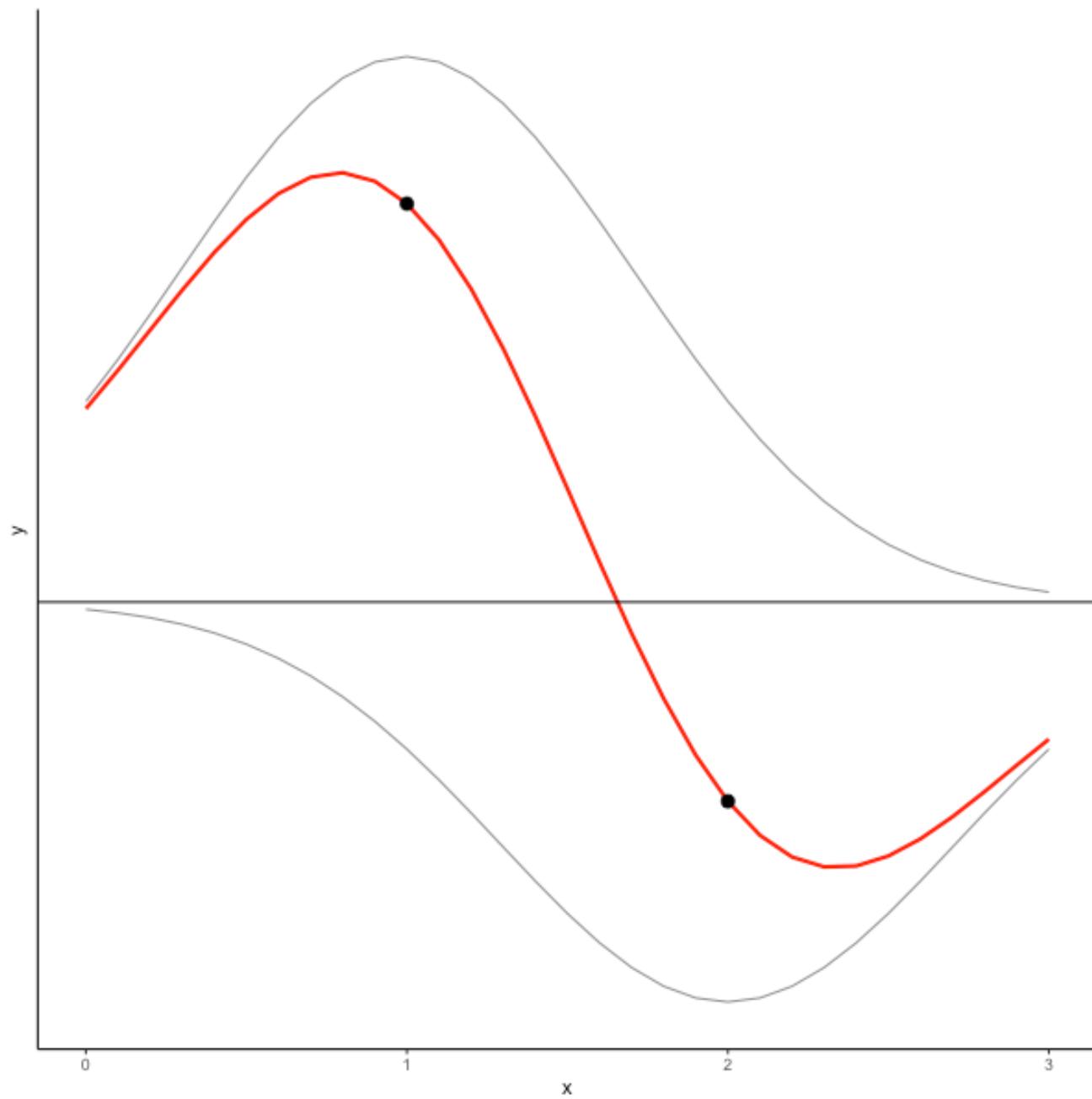
$$\int_A \hat{f}(x) dx =$$

Examples:

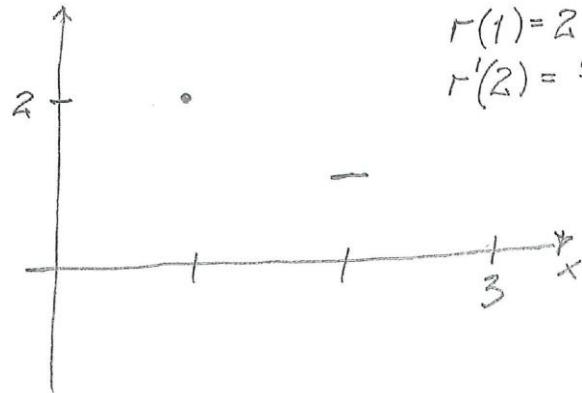
(A)



$$f(1) = 2$$
$$f(2) = -1$$



③



$$r(1) = 2$$
$$r'(2) = \frac{dr(x)}{dx} \Big|_{x=2} = 0$$

