Random fields and spatial priors

Janne Huttunen

UEF

November 10, 2015

Janne Huttunen (UEF)

Random fields and spatial priors

November 10, 2015

- Next we will give short introduction to stochastic processes and random fields
- Motivation: stochastic processes and random fields can be used for (for example):
 - **Dynamical or nonstationary inverse problems:** unknown and other quantities are temporally varying (functions of time).
 - **Spatial priors:** prior models for distributed unknown quantities (unknowns are functions of the spatial coordinate *x*).
- Spatial priors are presented at the end of this presentation
- Dynamical inverse problems and different solution methods are the subject of the rest of part 2 (lectures L17->).

Stochastic process

A stochastic process is a parametrized collection of random variables: $\{X(s)\}_{s\in\mathcal{D}}$ where \mathcal{D} is a set.

Usual terminology:

- Discrete process: $\mathcal{D} = \{0,1,2,\ldots\}$ (or some other discrete set)
- (Continuous time) stochastic process: D is a subset of real line ℝ and s is usually time: e.g. {X(t)}_{t≥0}
- Random field: D is a subset of R^d (d = 1, 2, ...) and the parameter s is a spatial coordinate x. Example: {X(x)}_{x∈S1}, where S_R = {x ∈ R³ : ||x|| = R} is a sphere in R³ (typical for modelling processes on the surface of Earth e.g. in climate)
- Space-time process: e.g. $\{X(t,x): t \ge 0, x \in D\}, D \subset \mathbb{R}^d$

Commonly the set \mathcal{D} is not specified in the notation if it is known from the context. The brackets are also often omitted and the process is simply denoted by X(s) or X(x). Notations X_k and X_t are also common for discrete and continuous time processes.

- In probability theory, random variables are defined as functions of ω ∈ Ω. Similarly stochastic processes can be considered as functions of s and ω: X(ω, s) or X(s, ω)
- Stochastic processes and random fields can also be thought as function valued random variables:
 - Random variables: realizations are real numbers: $X(\omega) \in \mathbb{R}$ when ω is fixed
 - Random vectors: realizations are vectors: $X(\omega) \in \mathbb{R}^n$ when ω is fixed
 - Stochastic processes and random fields: when ω is fixed, $X(\omega)$ is a function of the parameter s, that is, $s \to X(\omega, s)$,

Specify six functions

$$f^{1}(t) = t$$

$$f^{2}(t) = \sin(t),$$

$$f^{3}(t) = \log(t+1),$$

$$f^{4}(t) = t^{2} - t,$$

$$f^{5}(t) = \cos(t),$$

$$f^{6}(t) = 1.$$

Let $\omega \in \{1, ..., 6\}$ be an outcome of throwing a dice. We can specify a stochastic process by $X(\omega, t) = f^{\omega}(t)$.

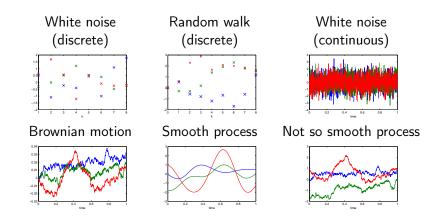


Figure: Examples of stochastic processes: red, green and blue are three different realizations of the process.

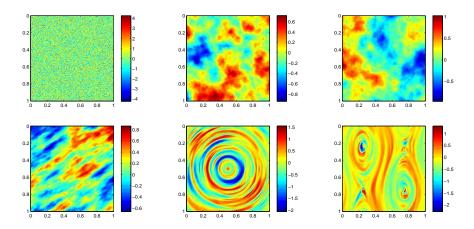


Figure: Realizations from different random fields (all Gaussian).

- The mean function: $\mu(s) = \mathbb{E}[X(s)], s \in \mathcal{D}$.
- The covariance function:

 $C(s,s') = \operatorname{cov}(X(s),X(s')) = \mathbb{E}\left[(X(s) - \mu(s))(X(s') - \mu(s'))\right]$ for $s,s' \in \mathcal{D}$.

• Note: $\operatorname{var}(X(s)) = \mathbb{E}\left[(X(s) - \mu(s))^2\right] = C(s, s).$

• *Finite dimensional joint-distributions*: let s_1, \ldots, s_n be a points in \mathcal{D} . The finite dimensional joint-distributions of a process X(s) are given by

$$F_{s_1,\ldots,s_n}(y_1,\ldots,y_n) = \mathbb{P}(X(s_1) \leq y_1,\ldots,X(s_n) \leq y_n)$$

for $y_1, \ldots, y_n \in \mathbb{R}$.

Stationary process

A process X(s) is called (strictly) *stationary* if for every set of points s_1, \ldots, s_n in \mathcal{D} , the finite dimensional joint-distributions are shift-invariant:

$$F_{s_1+h,\ldots,s_n+h}(y_1,\ldots,y_n)=F_{s_1,\ldots,s_n}(y_1,\ldots,y_n)$$

for all $h \in \mathcal{D}$ such that $s_i + h \in \mathcal{D}$.

Weakly stationary process

A process X(s) is called *weakly stationary* if for all s, s' and h:

$$\mu(s+h) = \mu(s)$$
 $C(s+h,s'+h) = C(s,s') = C(s-s').$

- In other words: weakly stationary process has the mean function which is a constant and the covariance is a only function of $\tau = s s'$, $C(\tau)$
- A strictly stationary process is also weakly stationary, opposite is not always true.

Isotriphic process

A process X(s) is called *isotrophic* if for all s, s':

$$C(s,s')=C(||s-s'||).$$

- In other words, the process is isotropic if the covariance function can be expresses as a function of the distance r = ||s s'|| (no directional dependency).
- Processes that are not isotrophic (i.e. the covariance depends on the direction) are called as anisotrophic.

Gaussian processes

The process is called Gaussian if $(X(s_1), \ldots, X(s_n))$ is a Gaussian random vector for all sets of points $s_1, \ldots, s_n \in D$.

- In other words, the process is Gaussian if all finite dimensional joint-distributions are Gaussian
- Gaussian processes are completely determined by the mean and covariance function
- Weakly stationary Gaussian processes are also strictly stationary
- GMRF: Gaussian Markov random field

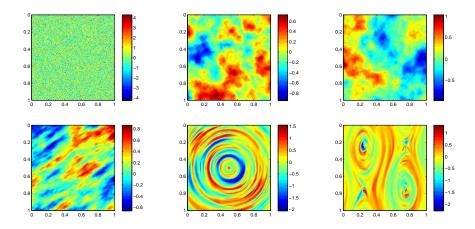


Figure: Realizations from Gaussian random fields. Top row: white noise (left) and two realizations of a same isotrophic random field (middle and right). Bottom row: a realization of an anisotrophic random field (left), and two different nonstationary random fields (middle, right).

• The following Markov property is useful with Kalman filters (dynamic inverse problems):

Markov property for a discrete process

A discrete process X_k has so called Markov property, if the conditional probability distribution of X_k given all states X_s , s < k, equals to the conditional probability distribution of X_k given the previous state X_{k-1} :

$$p(x_k|x_s, s < k) = p(x_k|x_{k-1})$$

In other words, if X_{k-1} is known, the knowledge of X_{k-2}, X_{k-3}, \ldots does provide any additional information about the current state X_k

• Markov property can also be given for continuous processes and random fields (omitted in this course).

- Often unknown quantities are modelled as Gaussian variables since Gaussian distributions leads to computational efficient problems, or we just do not know any better distribution for the variable
- From now on we only consider Gaussian random fields
- When we consider Gaussian random fields, we only need to think about the mean and covariance function

- The mean can be chosen based on the prior information related to the problem.
- Often the mean function is written a sum of functions basis ϕ_i functions:

$$\mu(s) = \sum_i \theta_i \phi_i(s)$$

for which the coefficients θ_i are determined based on some sort of data (e.g. hyper parameters in inverse problems).

• The form of basis functions is chosen based on the application: e.g. piecewise linear functions, polynomials, sin and cos functions (wave propagation problems).

- In principle the form of the covariance function could be chosen to be a function of s and s' which can also include some parameters (e.g. variance and scaling parameters) that are determined based on data
- However the covariance function should satisfy some requirements implied by the definition
- Furthermore, some attention should be paid to check that the random field will have preferred continuity and smoothness properties

Requirements for covariance functions

- First of all, C has to be symmetric: C(s, s') = C(s', s) for all $s, s' \in \mathcal{D}$. For stationary process: $C(\tau) = C(-\tau)$ where $\tau = s s'$.
- Furthermore, consider a set of points {s_i ∈ D : i = 1,..., n} and let K be a n × n matrix such that the elements are

$K_{ij} = C(s_i, s_j), \quad i, j = 1, \dots, n$

- If C is the covariance function of a process X, the matrix K is the covariance matrix of the n-dimensional random vector (X(s₁),...,X(s_n)).
- All covariance matrices should be positive semidefinite: x^T Kx ≥ 0 for all vectors x ∈ ℝⁿ
- Therefore the covariance function has to be positive semidefinite: for all set of points $\{s_1, \ldots, s_n\} \subset D$, the matrix K given above is positive semidefinite.

Continuity and smoothness

- A stochastic process X is continuous in mean square at s_{*} if and only if C(s, s') is continuous at s = s' = s_{*}. For stationary X, it is sufficient to check continuity of C(τ) at τ = 0.
- The derivates of C determines the smoothness of X: if ^{∂²C(s,s')}/_{∂s_i∂s'_i} exists and is finite, ^{∂X}/_{∂s_i} exists (in mean square sense) and its covariance function is ^{∂²C(s,s')}/_{∂s_i∂s'_i}. Higher order derivatives similarly.
 Stationary X: if ^{∂^{2k}C(τ)}/_{∂d^{2k}} exists and is finite at τ = 0, the derivative ^{∂^kX}/_{∂s^k} exists (in mean square sense).

Summary (what should be remembered from the slide)

The continuity and smoothness of X are determined by the continuity and smoothness of the covariance function at s = s' at $\tau = 0$. Janne Huttunen (UEF) Random fields and spatial priors November 10, 2015 19 / 43

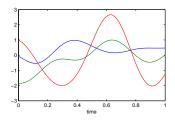
Squared exponential covariance function

Squared exponential covariance function:

$$\mathcal{C}(au) = \exp\left(-rac{\| au\|^2}{2\ell^2}
ight)$$

where $\ell > 0$ is scaling parameter often called as *characteristic length-scale*.

- Simple form and very widely used
- C(τ) is infinitely differentiable
 ⇒ X has mean square derivates of all orders and thus very smooth
- Such very strong smoothness properties may be unrealistic in many applications



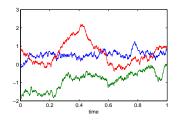
Janne Huttunen (UEF)

Exponential covariance function

Exponential covariance function is of the form

$$\mathcal{C}(au) = \exp\left(-rac{\| au\|}{\ell}
ight)$$

- C continuous but not differentiable at $\tau = 0 \Rightarrow$ the process is continuous in mean square, but not differentiable
- May be too rough process for many applications (especially if smoothness is preferred)



Mátern class of covariance functions

Mátern class of covariance functions is given by

$$C_{\nu}(\tau) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu} \|\tau\|}{\ell}\right)^{\nu} K_{\nu}\left(\frac{\sqrt{2\nu} \|\tau\|}{\ell}\right)$$

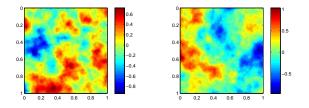
where ν and ℓ are positive parameters and ${\it K}_{\nu}$ is the modified Bessel function of second order.

- The parameter ν determines the smoothness properties of the process: the process is k'th times mean square differentiable if and only if $\nu > k$.
- Furthermore, the limit $\nu \to \infty$ gives the squared exponential covariance function, $\nu = \frac{1}{2}$ gives the exponential covariance function.

Examples of covariance functions

 For other half integers ν = p + ¹/₂ (p > 0), the Matérn covariance functions are products of an exponential function and a polynomial of order p:

$$\begin{aligned} \mathcal{C}_{\nu=\frac{3}{2}}(\tau) &= \left(1 + \frac{\sqrt{3} \|\tau\|}{\ell}\right) \exp\left(-\frac{\sqrt{3} \|\tau\|}{\ell}\right) \\ \mathcal{C}_{\nu=\frac{5}{2}}(\tau) &= \left(1 + \frac{\sqrt{5} \|\tau\|}{\ell} + \frac{5 \|\tau\|^2}{3\ell^2}\right) \exp\left(-\frac{\sqrt{5} \|\tau\|}{\ell}\right) \end{aligned}$$



Janne Huttunen (UEF)

Random fields and spatial priors

November 10, 2015

- The covariances functions can be also formed as combination of several covariance function:
 - The sum of two covariance functions is also a valid covariance function (the covariance function of $X_1(s) + X_2(s)$ of when X_1 and X_2 are independent)
 - The product of two covariance functions is also a valid covariance function (the covariance function of $X_1(s)X_2(s)$ when X_1 and X_2 are independent). Thus also $C(s, s')^p$ is a valid covariance function.
 - Let a(s) be a deterministic function. Then the covariance function of Y(s) = a(s)X(s) is a(s)C(s,s')a(s') if C is the covariance function of the process X(s).

- All of the above covariance functions are stationary and isotropic, and normalized such that C(0) = var(X(s)) = 1.
- Sometimes we may want more flexibility and, for example, choose the variance as a function of s, $\sigma(s)$. Then we can write e.g.:

$$X(s) = \mu(s) + \sigma(s)X'(s)$$

and consider the construction of X'(s) as a stationary process.

• If the covariance of X'(s) is C'(s, s'), the covariance of X is $C(s, s') = \sigma(s)\sigma(s')C'(s, s')$ (as in the previous slide)

- The above correlation functions can be modified for anisotrophical cases (correlation different to different directions) easily.
- We consider only stationary two-dimensional case, other dimensions are similar
- The previous isotrophic correlation functions include the term $\|\tau\|/\ell = \sqrt{\frac{\tau_x^2}{\ell^2} + \frac{\tau_y^2}{\ell^2}}$ where $\tau = (\tau_x, \tau_y)$
- To introduce different characteristic length-scales to the x and y-direction, we can replace this terms with $\sqrt{\frac{\tau_x^2}{\ell_x^2} + \frac{\tau_y^2}{\ell_y^2}}$
- For example, anisotrophic squared exponential covariance function:

$$C(\tau) = \exp\left\{-\frac{1}{2}\left(\frac{\tau_x^2}{\ell_x^2} + \frac{\tau_y^2}{\ell_y^2}\right)\right\}$$

Anisotrophic covariance functions

- Other directions can be handled using coordinate transformations
- Note that

$$\frac{\tau_x^2}{\ell_x^2} + \frac{\tau_y^2}{\ell_y^2} = \tau^{\mathrm{T}} \Lambda \tau, \quad \Lambda = \mathrm{diag}(\ell_x^{-2}, \ell_y^{-2}).$$

• We apply an coordinate transform matrix *C* and replace the term with

 $\tau^{\mathrm{T}} \mathcal{C} \Lambda \mathcal{C}^{\mathrm{T}} \tau$

• E.g. C can be a rotation matrix

$$C = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$$

which rotates points in xy-plane counter-clockwise with an angle θ

0.8 0.6 0.2 0.4 0.4 0.2 0 0.6 -0.2 0.8 -04 -0.6 ່ດ 02 04 06 0.8 1

Janne Huttunen (UEF)

- Random fields can be applied for interpolation of a function as follows.
- For example, we have an unknown function $X : [0,1] \mapsto \mathbb{R}$.
- We have observations of X at a given set of points $x_1, \ldots, x_n \in [0, 1]$: $y_i = X(x_i), i = 1, \ldots, n$.
- We want to estimate the value of X in an arbitrary point $x_0 \in [0, 1]$ (interpolation).

Example: stochastic interpolation (Kriging)

- We model X as a Gaussian random field.
- In this example, we choose $\mu(s) = 0$ and C is the Matérn covariance function with $\nu = 3/2$
- Define random variables $\mathbf{X} = X(x_0)$ and $\mathbf{Y} = (y_1, \dots, y_n)^{\mathrm{T}} = (X(x_1), \dots, X(x_n))^{\mathrm{T}}.$
- Since X and Y are jointly Gaussian random variables, the conditional distribution of X given Y is Gaussian: $\mathcal{N}(\hat{X}, \sigma_{X|Y}^2)$ where

$$\hat{\mathbf{X}} = \bar{\mathbf{X}} + \Gamma_{\mathbf{XY}}\Gamma_{\mathbf{Y}}^{-1}(\mathbf{Y} - \bar{\mathbf{Y}}) \sigma_{\mathbf{X}|\mathbf{Y}}^2 = \sigma_{\mathbf{X}}^2 - \Gamma_{\mathbf{XY}}\Gamma_{\mathbf{Y}}^{-1}\Gamma_{\mathbf{XY}}^{\mathrm{T}}$$

(see the preliminaries PDF)

The above equations gives our solution: the mean X̂ gives an estimate for X(x₀) and σ²_{X|Y} is an estimate of its uncertainty (variance). For interpolation, we can vary x₀.

Janne Huttunen (UEF)

Example: stochastic interpolation (Kriging)

- Before we can use the above equations, we need to calculate the expectations of X and Y, the variance σ_{X}^{2} , the covariance Γ_{Y} and the cross-covariance Γ_{XY}
- The expectations are given by the mean function: $\bar{\mathbf{X}} = \mu(x_0) = 0$ and $\bar{\mathbf{Y}} = (\mu(x_1), \dots, \mu(x_n))^T = 0$
- The variance of **X** is $\sigma_X^2 = C(x_0, x_0)$
- The covariance of Y is the matrix Γ_Y which elements are C(x_i, x_j) (i, j = 1,..., n)
- The cross-covariance of X and Y is $\Gamma_{XY} = (C(x_0, x_1), \dots, C(x_0, x_n))$
- Note: it is easy to expand the approach for noise-corrupted measurements y_i = X(x_i) + ε_i, where ε ~ N(0, σ_ε²I) independent of X. In this case Γ_Y in the above formulae is replaced with Γ_Y + σ_ε²I.

Example: stochastic interpolation

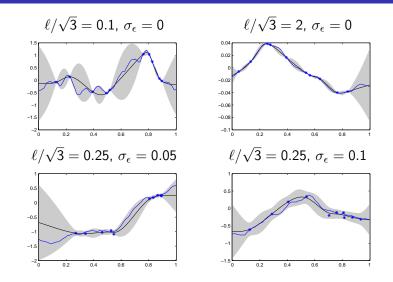


Figure: Stochastic interpolation: the blue line is the true function f and the black line is the estimate. The gray band corresponds to 2xS.D. error limits. Starts

Janne Huttunen (UEF)

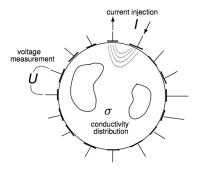
Random fields and spatial priors

November 10, 2015

- **Spatial priors:** prior models inverse problems in which unknowns depend on the spatial coordinate *x* (e.g. heterogeneous variables).
 - Unknown quantities are modelled as random fields
 - The prior distribution is given by the distribution of random field.
 - If can be assumed to be Gaussian:
 ⇒ specify the mean and covariance function

Example: Electrical impedance tomography (EIT)

- Unknown (electric) conductivity distribution σ(x) is a heterogenous variable
- We want to determine σ (e.g. tomographic imaging)
- Electrodes on boundary
- Inject electric currents *I* → measure voltages *U*
- Problem: reconstruct σ from
 (I, U) information



- Consider an inverse problem in which unknown X(x) is a spatially varying function (distributed parameter, a heterogeneous variable)
- X(x) can be modelled as a random field
- To specify a Gaussian prior: specify mean function $\mu(x)$ and covariance function C(x, x')
- The mean $\mu(x)$ is specified based on prior information related to the application
- For the covariance function C(x, x') can be chosen to be, for example, one of the listed previously based on the prior knowlege. For example:
 - $\bullet\,$ expected to be very smooth \rightarrow squared exponential
 - $\bullet~\mbox{expected}$ to non-smooth $\rightarrow~\mbox{exponential}$
 - Matérn if between those

- The inverse problem is usually discretized numerically for practical implementation (e.g. finite difference method, finite element method)
- The discretized unknown often represents the unknown X(x) in a grid of points.
- Let $\{x_i, i = 1, ..., n\}$ be such grid points.
- Then prior can be chosen as $\mathcal{N}(\mu,\mathbf{\Gamma})$ where

$$\mu = (\mu(x_1), \dots, \mu(x_n))^{\mathrm{T}}$$

$$\Gamma(i, j) = C(x_i, x_j), \quad i, j = 1, \dots, n.$$

- Sometimes the expected variance of the field can also depend on the spatial variable
- We could specify a non-stationary covariance
- However, it is usually easier to work with stationary covariances and, for example, specify X as

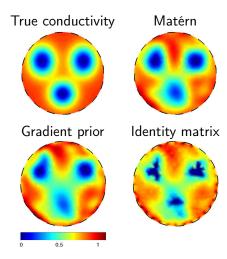
$$X(x) = \mu(x) + \sigma(x)W(x)$$

where $\sigma(x)$ is preferred variance (also chosen based on the problem) and W is a stationary random field (zero mean)

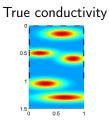
- The stationary covariance is specified for W
- Then $C_X(x,x') = \sigma(x)C(x,x')\sigma(x')$ and

$$\mathbf{\Gamma}(i,j) = \sigma(x_i) C(x_i, x_j) \sigma(x_j)$$

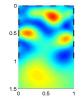
Electrical impedance tomography in a circular tank



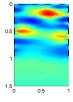
Ground prospecting with anisotropic conductivities



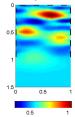
Isotropic Mátern



Anisotropic gradient



Anisotropic Mátern



- Priors can include parameters that are not precisely known
- \bullet For example: mean, variance, length-scale ℓ
- We can model these as hierarchical prior parameters often called as hyperparameters:
 - Consider such parameters also as unknown in the inverse problems
 - Write a prior model for the hyper parameters
 - Consider both the primary unknown X and the hyper parameters as unknown and estimate it from the data

We consider an example:

• Assume that the mean is presented using basis functions θ_i

$$\mu(x) = \sum_{i=1}^{p} \gamma_i \phi_i(x)$$

where γ_i are unknown.

- Assume that the variance σ^2 (assumed to be a constant) and the length-scale ℓ in the covariance function are also unknown
- We denote the vector of hyper parameters by θ :

$$\theta = (\gamma_1, \ldots, \gamma_p, \sigma^2, \ell)$$

Example of hierarchical models

- Discretization: X presented at points x_1, \ldots, x_n
- For discretized prior mean: $\mu_X = (\mu(x_1), \dots, \mu(x_n))^{\mathrm{T}} = \Phi \gamma$ where

$$\Phi = \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_1(x_n) \\ \vdots & \ddots & \vdots \\ \phi_p(x_1) & \cdots & \phi_p(x_n) \end{pmatrix}, \quad \gamma = \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_p \end{pmatrix}$$

The prior model:

$$\pi(X, heta)=\pi(X| heta)\pi(heta)$$

where

$$\pi(X|\theta) \propto e^{-\frac{1}{2}\left[(X-\Phi\gamma)^{\mathrm{T}} \Gamma_X^{-1}(\sigma^2,\ell)(X-\Phi\gamma) + \log \det(\Gamma_X(\sigma^2,\ell))\right]}$$

The log term is due to the normalization constant (which now depends on the unknown hyperparameters and has to be included).

Janne Huttunen (UEF)

- The hyperprior $\pi(\theta)$ is specified by using prior knowledge/beliefs of hyper parameters.
- For example: $\gamma \sim \mathcal{N}(0, \Gamma_{\gamma})$ with known Γ_{γ}
- Inverses of the variances are often modelled using Gamma distributions:

$$\pi(\sigma^{-2}) = \operatorname{Gamma}(\alpha_{\sigma}, \beta_{\sigma}) \quad \text{or} \quad \pi(\sigma^{2}) = \operatorname{InvGamma}(\alpha_{\sigma}, \beta_{\sigma})$$
$$\Rightarrow \pi(\sigma^{2}) \propto (\sigma^{2})^{-\alpha_{\sigma}-1} e^{-\beta_{\sigma}/\sigma^{2}} = e^{-\beta_{\sigma}/\sigma^{2} - (\alpha_{\sigma}+1)\log\sigma^{2}}$$

• The scale length parameter can be chosen to follow, for example, Gamma distribution

$$\pi(\ell) \propto \ell^{lpha_\ell - 1} e^{-eta_\ell \ell} = e^{-eta_\ell \ell - (1 - lpha_\ell) \log \ell}$$

• Usually the hyper parameters are assumed to be independent:

$$\pi(\theta) = \pi(\gamma)\pi(\sigma^2)\pi(\ell)$$

- The posterior is $\pi(X, \theta | m) \propto \pi(m | X) \pi(X | \theta) \pi(\theta)$
- If we have an observation model m = A(x) + ε, ε ~ N(0, Γ_ε), the posterior for our example is

$$\begin{split} &-\log \pi(X,\theta|m) \\ &= \frac{1}{2}(m-A(x))^{\mathrm{T}} \Gamma_{\epsilon}^{-1}(m-A(x)) \\ &+ \frac{1}{2} \left(X - \Phi \gamma\right)^{\mathrm{T}} \Gamma_{X}^{-1}(\sigma^{2},\ell) \left(X - \Phi \gamma\right) + \frac{1}{2} \log \det(\Gamma_{X}(\sigma^{2},\ell)) \\ &+ \frac{1}{2} \gamma^{\mathrm{T}} \Gamma_{\gamma}^{-1} \gamma + \beta_{\sigma} / \sigma^{2} + (\alpha_{\sigma}+1) \log \sigma^{2} + \beta_{\ell} \ell + (1 - \alpha_{\ell}) \log \ell \ell \end{split}$$

- The above function can be minimized using optimization algorithms (e.g. Gauss-Newton) to compute MAP estimate, or use MCMC methods for CM estimates.
- Furthermore, if the posterior is simple, the hyper parameters could perhaps be integrated out to obtain $\pi(X|m)$