# ADVANCED BAYESIAN LEARNING GAUSSIAN PROCESSES Spring 2014

Mattias Villani

Division of Statistics

Department of Computer and Information Science
Linköping University

#### TOPIC OVERVIEW

- Gaussian process regression
  - ► Recall: Bayesian inference for Gaussian linear/nonlinear regression.
  - ► Gaussian processes for nonparametric regression
  - Covariance kernels
  - Properties of GPs
  - Selecting the kernel and hyperparameters
- ► Gaussian process classification
  - Flexible classification using GPs
  - Laplace approximation of the posterior
- ▶ Main literature: Rasmussen and Williams (2006). *Gaussian Processes* for Machine Learning.

#### FLEXIBLE NONLINEAR REGRESSION

► Linear regression

$$y = f(\mathbf{x}) + \epsilon$$
$$f(\mathbf{x}) = \mathbf{x}^T \cdot \mathbf{w}$$

and  $\epsilon \sim N(0, \sigma_n^2)$  and iid over observations.

- ▶ The weights **w** are called regression coefficients ( $\beta$ ) in statistics.
- ▶ Polynomial regression:  $\mathbf{x} = (1, x, x^2, x^3, ..., x^k)^T$ .
- ► Spline regression:

$$f(\mathbf{x}) = \phi(\mathbf{x})^T \cdot \mathbf{w}$$

where  $\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), ..., \phi_N(\mathbf{x}))^T$  for N basis functions

**Example:** thin plate splines with N knots  $\kappa_1, ..., \kappa_N$  in x-space

$$\phi_k(\mathbf{x}) = \ln \left( \|\mathbf{x} - \kappa_k\| \right) \|\mathbf{x} - \kappa_k\|^2$$

## BAYESIAN LINEAR REGRESSION - INFERENCE

- ightharpoonup w is unknown.  $\sigma_n$  is assumed known.
- Prior [note: RW do not use  $\Sigma_p = \sigma_n^2 \Omega$ ]

$$\mathbf{w} \sim N\left(0, \Sigma_{p}\right)$$

**Posterior** [note: X is  $D \times n$ ]

$$\begin{split} \mathbf{w}|\mathbf{X}, &\mathbf{y} \sim \mathcal{N}\left(\bar{\mathbf{w}}, \mathbf{A}^{-1}\right) \\ \mathbf{A} &= \sigma_n^{-2} \mathbf{X} \mathbf{X}^T + \Sigma_p^{-1} \\ \bar{\mathbf{w}} &= \sigma_n^{-2} \mathbf{A}^{-1} \mathbf{X} \mathbf{y} = \left(\mathbf{X} \mathbf{X}^T + \sigma_n^2 \Sigma_p^{-1}\right)^{-1} \mathbf{X} \mathbf{y} \end{split}$$

- ► Recall: Posterior precision = Data Precision + Prior Precision.
- Marginal posterior of **w** is multivariate student-t when  $\sigma_n^2$  is unknown with Inv- $\chi^2$  prior (and  $\Sigma_p = \sigma_n^2 \Omega$ ).

#### **BAYESIAN LINEAR REGRESSION - PREDICTION**

▶ Predictive density for mean  $f(x_*)$  at new location  $x_*$ 

$$f(\mathbf{x}_*)|\mathbf{x}_*, \mathbf{X}, \mathbf{y} \sim N\left(\mathbf{x}_*^T \bar{\mathbf{w}}, \mathbf{x}_*^T \mathbf{A}^{-1} \mathbf{x}_*\right)$$

▶ Proof:  $f(\mathbf{x}_*) = \mathbf{x}_*^T \mathbf{w}$  and  $\mathbf{w}$  has a normal posterior. Linear combs of normals is normal.

► Predictive density for new response y<sub>\*</sub>

$$\mathbf{y}_* | \mathbf{x}_*, \mathbf{X}, \mathbf{y} \sim \mathcal{N}\left(\mathbf{x}_*^T \bar{\mathbf{w}}, \mathbf{x}_*^T \mathbf{A}^{-1} \mathbf{x}_* + \sigma_n^2\right)$$

▶ Replace **X** with  $\Phi(\mathbf{X})$  in the above for the case with basis expansion (e.g. splines).

#### NON-PARAMETRIC REGRESSION

Non-parametric regression: avoiding a parametric form for  $f(\cdot)$ . Treat  $f(\mathbf{x})$  as an unknown parameter for every  $\mathbf{x}$ .

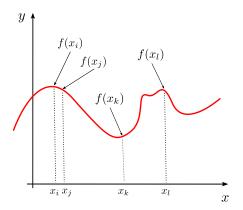
#### ► Weight space view

- ▶ Restrict attention to a grid of (ordered) x-values:  $x_1, x_2, ..., x_k$ .
- ▶ Put a joint prior on the k function values:  $f(x_1), f(x_2), ..., f(x_k)$ .

#### ► Function space view

- ► Treat f as an unknown function.
- Put a prior over a set of functions.
- ► Kolmogorov's existence theorem for stochastic processes equates the two views. Just make sure that the set of finite dimensional distributions are consistent: adding or deleting variables does not change the marginal of the original variable set.

# NONPARAMETRIC = ONE PARAMETER FOR EVERY X!



#### THE MULTIVARIATE NORMAL DISTRIBUTION

▶ The **density function** of a *p*-variate normal vector  $\mathbf{x} \sim N(\mu, \Sigma)$  is

$$f(\mathbf{x}) = \left(\frac{1}{2\pi}\right)^{p/2} \frac{1}{\sqrt{\det \Sigma}} \exp\left\{-\frac{1}{2}(\mathbf{x} - \mu)' \Sigma^{-1}(\mathbf{x} - \mu)\right\}$$

▶ Example: **Bivariate normal** (p = 2)

$$\Sigma = \left( egin{array}{cc} \sigma_1^2 & 
ho\sigma_1\sigma_2 \ 
ho\sigma_1\sigma_2 & \sigma_2^2 \end{array} 
ight)$$

▶ Linear combinations. Let y = Bx + b, where x is  $p \times 1$  and B is a  $m \times p$  constant matrix. Then

$$\mathbf{y} \sim N(\mathbf{B}\mu + \mathbf{b}, \mathbf{B}\Sigma\mathbf{B}')$$

# THE MULTIVARIATE NORMAL DISTRIBUTION, CONT.

- Let  $\mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}$  where  $\mathbf{x}_1$  is  $p_1 \times 1$  and  $\mathbf{x}_2$  is  $p_2 \times 1$   $(p_1 + p_2 = p)$ .
- ightharpoonup Partition  $\mu$  and  $\Sigma$  accordingly as

$$\mu=\left(egin{array}{c} \mu_1 \ \mu_2 \end{array}
ight)$$
 and  $\Sigma=\left(egin{array}{cc} \Sigma_{11} & \Sigma_{12} \ \Sigma_{21} & \Sigma_{22} \end{array}
ight)$ 

▶ Marginals are normal. Let  $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$ , then

$$\mathbf{x}_1 \sim N(\mu_1, \Sigma_{11})$$

▶ Conditionals are normal. Let  $\mathbf{x} \sim N(\mu, \Sigma)$ , then

$$\mathbf{x}_1 | \mathbf{x}_2 = \mathbf{x}_2^* \sim N \left[ \mu_1 + \Sigma_{12} \Sigma_{22}^{-1} (\mathbf{x}_2^* - \mu_2), \ \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \right]$$

► Life is beautiful ...

#### GAUSSIAN PROCESS REGRESSION

▶ Weight-space view. GP assumes

$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{pmatrix} \sim N(\mathbf{m}, \mathbf{K})$$

▶ But how do we specify the  $k \times k$  covariance matrix K?

$$Cov\left(f(x_p),f(x_q)\right)$$

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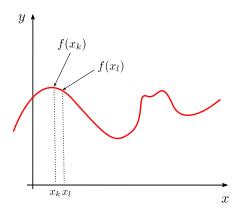
$$Cov\left(f(x_p),f(x_q)\right)$$

Squared exponential covariance function

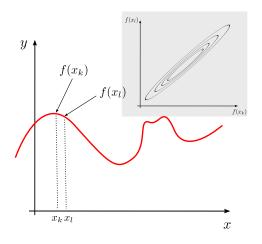
Cov 
$$(f(x_p), f(x_q)) = k(x_p, x_q) = \sigma_f^2 \exp\left(-\frac{1}{2}(x_p - x_q)^2\right)$$

- ▶ Nearby x's have highly correlated function ordinates f(x).
- ▶ We can compute  $Cov(f(x_p), f(x_q))$  for any  $x_p$  and  $x_q$ .
- ▶ Extension to multiple covariates:  $(x_p x_q)$  replaced by  $\|\mathbf{x}_p \mathbf{x}_q\|$ .

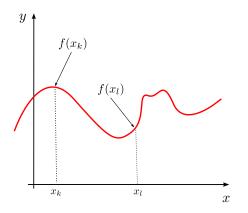
# SMOOTH FUNCTION - POINTS NEARBY



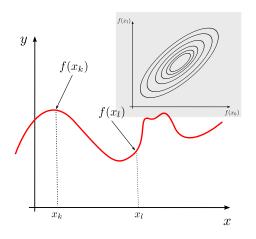
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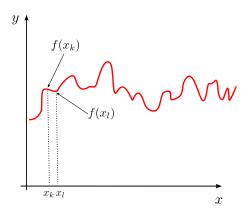
## SMOOTH FUNCTION - POINTS FAR APART



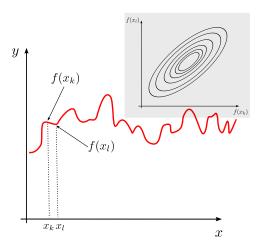
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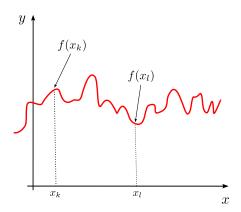
# JAGGED FUNCTION - POINTS NEARBY



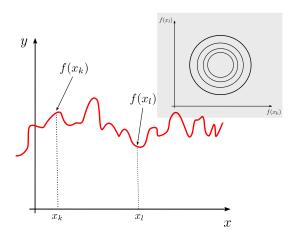
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# JAGGED FUNCTION - POINTS FAR APART



# GAUSSIAN PROCESS REGRESSION, CONT.

#### **DEFINITION**

A Gaussian process (GP) is a collection of random variables, any finite number of which have a multivariate Gaussian distribution.

- ► A Gaussian process is really a **probability distribution over functions** (curves). No need for a grid!
- ► A GP is completely specified by a **mean** and a **covariance function**

$$m(x) = \mathbb{E}[f(x)]$$
$$k(x, x') = \mathbb{E}[(f(x) - m(x)) (f(x') - m(x'))]$$

for any two inputs x and x' (note: this is *not* the transpose here).

► A Gaussian process is denoted by

$$f(x) \sim GP(m(x), k(x, x'))$$

**Bayesian**:  $f(x) \sim GP$  encodes **prior beliefs** about the unknown  $f(\cdot)$ .

#### A SIMPLE GP EXAMPLE

► Example:

$$m(x) = \sin(x)$$
  $k(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2}\left(\frac{x - x'}{\ell}\right)^2\right)$ 

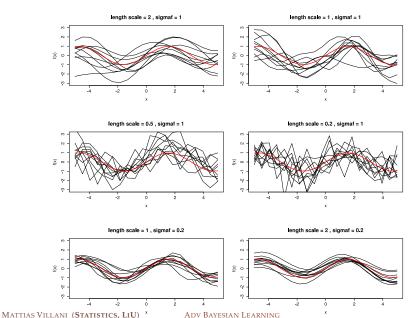
where  $\ell > 0$  is the length scale.

- ▶ Larger  $\ell$  gives more smoothness in f(x).
- ▶ Simulate draw from  $f(x) \sim GP(m(x), k(x, x'))$  over a grid  $\mathbf{x}_* = (x_1, ..., x_n)$  by using that

$$f(\mathbf{x}_*) \sim N(m(\mathbf{x}_*), K(\mathbf{x}_*, \mathbf{x}_*))$$

Note that the **kernel** k(x, x') produces a **covariance matrix**  $K(\mathbf{x}_*, \mathbf{x}_*)$  when evaluated at the vector  $\mathbf{x}_*$ .

# SIMULATING A GP - SINE MEAN AND SE KERNEL



## SIMULATING A GP

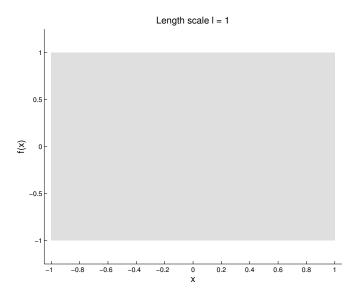
▶ The joint way: Choose a grid  $x_1, ..., x_k$ . Simulate the k-vector

$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_k) \end{pmatrix} \sim N(\mathbf{m}, \mathbf{K})$$

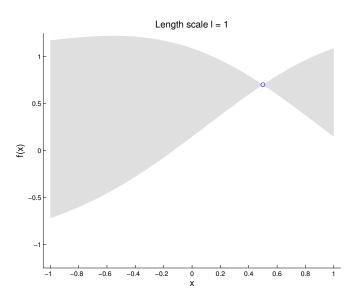
More intuition from the conditional decomposition

$$p(f(x_1), f(x_2), ...., f(x_k)) = p(f(x_1)) p(f(x_2)|f(x_1)) \cdots \times p(f(x_k)|f(x_1), ..., f(x_{k-1}))$$

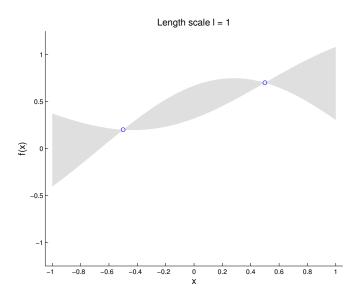
## DENSITY BEFORE FIRST DRAW



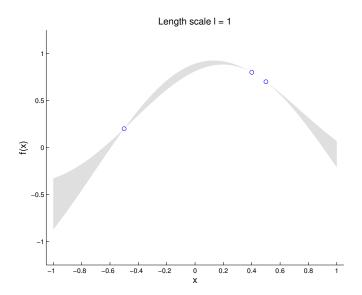
## DENSITY BEFORE SECOND DRAW



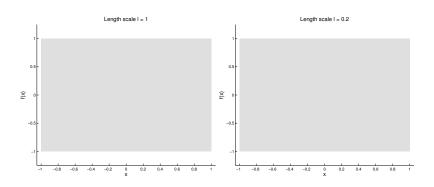
## DENSITY BEFORE THIRD DRAW



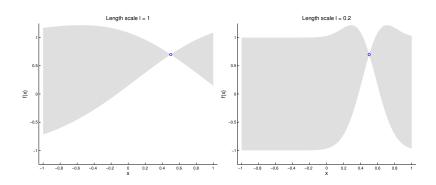
## DENSITY BEFORE FOURTH DRAW



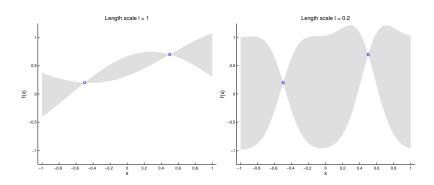
# SIMULATION FROM L=1 VS L=0.2. BEFORE FIRST DRAW.



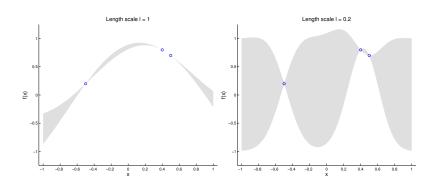
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# SIMULATION FROM L=1 VS L=0.2. BEFORE THIRD DRAW.



# SIMULATION FROM L=1 VS L=0.2. BEFORE FOURTH DRAW.



#### THE POSTERIOR FOR A GPR

Model

$$y_i = f(x_i) + \varepsilon_i, \quad \varepsilon \stackrel{iid}{\sim} N(0, \sigma^2)$$

► Prior

$$f(x) \sim GP(0, k(x, x'))$$

- ▶ You have observed the data:  $\mathbf{x} = (x_1, ..., x_n)'$  and  $\mathbf{y} = (y_1, ..., y_n)'$ .
- ▶ Goal: the posterior of  $f(\cdot)$  over a grid of x-values:  $\mathbf{f}_* = \mathbf{f}(\mathbf{x}_*)$ .

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- ► Intermediate step: joint distribution of y and f\*\*

$$\left(\begin{array}{c} y \\ f_* \end{array}\right) \sim \textit{N}\left\{\left(\begin{array}{c} 0 \\ 0 \end{array}\right), \left[\begin{array}{ccc} \textit{K}(x,x) + \sigma^2\textit{I} & \textit{K}(x,x_*) \\ \textit{K}(x_*,x) & \textit{K}(x_*,x_*) \end{array}\right]\right\}$$

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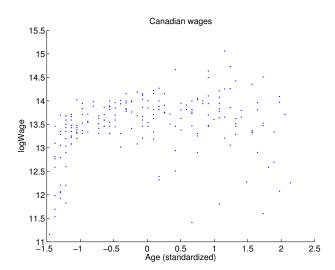
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► The posterior

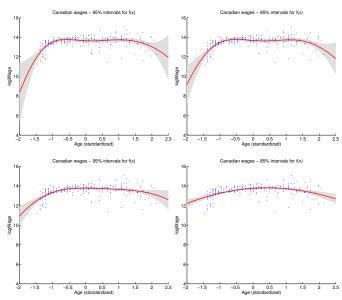
$$f_*|x, y, x_* \sim N\left(f_*, cov(f_*)\right)$$

$$\begin{split} \mathbf{\bar{f}}_* &= \mathcal{K}(\mathbf{x}_*, \mathbf{x}) \left[ \mathcal{K}(\mathbf{x}, \mathbf{x}) + \sigma^2 I \right]^{-1} \mathbf{y} \\ &\operatorname{cov}(\mathbf{f}_*) = \mathcal{K}(\mathbf{x}_*, \mathbf{x}_*) - \mathcal{K}(\mathbf{x}_*, \mathbf{x}) \left[ \mathcal{K}(\mathbf{x}, \mathbf{x}) + \sigma^2 I \right]^{-1} \mathcal{K}(\mathbf{x}, \mathbf{x}_*) \end{split}$$

# EXAMPLE - CANADIAN WAGES



# Posterior of F - $\ell = 0.2, 0.5, 1, 2$



## PREDICTION AND DECISION

lacktriangle Predicting a new set of y-values  $oldsymbol{y}_* = f(oldsymbol{x}_*) + \epsilon$  is easy

$$\mathbf{y}_* | \mathbf{x}, \mathbf{y}, \mathbf{x}_* \sim N\left(\overline{\mathbf{f}}_*, \operatorname{cov}(\mathbf{f}_*) + \sigma_n^2 I\right)$$

 $\triangleright$  Choosing a point prediction  $y_{guess}$  by maximizing expected utility

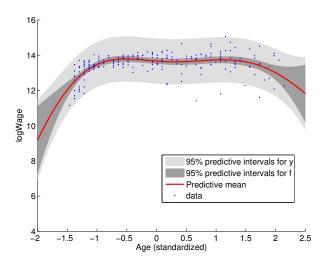
$$\bar{\mathcal{U}}(\mathbf{y}_{guess}|\mathbf{x}_*) = \int \mathcal{U}(\mathbf{y}_*, \mathbf{y}_{guess}) \rho(\mathbf{y}_*|\mathbf{x}_*, \mathbf{y}, \mathbf{x}) d\mathbf{y}_*$$

▶ Have to make a decision  $a \in \mathcal{A}$  whose consequences (utility) depends on the uncertain  $\mathbf{f}_*$  (or  $\mathbf{y}_*$ )? Just maximize expected utility

$$ar{\mathcal{U}}(\mathsf{a}) = \int \mathcal{U}(\mathsf{a},\mathsf{f}_*) 
ho(\mathsf{f}_*|\mathsf{x}_*,\mathsf{y},\mathsf{x}) d\mathsf{f}_*$$

where  $\mathcal{U}(a,\mathbf{f}_*)$  is the utility of action  $a\in\mathcal{A}$  if  $\mathbf{f}_*$  turns out to be the "true state of the world".

## Canadian wages - Prediction with $\ell=0.5$



## STATIONARY PROCESSES AND SMOOTHNESS

A stochastic process (field)  $\{f(\mathbf{x}), x \in \mathbb{R}^D\}$  is weakly stationary if  $E(f(\mathbf{x})) = \mu$  and its covariance function  $k(\mathbf{x}, \mathbf{x}')$  is a function of  $\mathbf{t} = \mathbf{x} - \mathbf{x}'$ 

$$k(\mathbf{x}, \mathbf{x}') = Cov[f(\mathbf{x}), f(\mathbf{x}')] = k(\mathbf{t}).$$

The covariance function is **isotropic** if it only depends on the distance  $t = \|\mathbf{x} - \mathbf{x}\|$  (invariant to directions)

$$k(\mathbf{x}, \mathbf{x}') = Cov [f(\mathbf{x}), f(\mathbf{x}')] = k(t).$$

- ► The **smoothness** of a stationary process is determined by the smoothness of the covariance function.
- ► A stationary (isotropic) process is continuous in quadratic mean

$$E\left(\left|f(\mathbf{x}+t)-f(\mathbf{x})\right|^2\right) o 0 \text{ as } t o 0$$

iff k(t) is continuous at t = 0.

A little more is required to guarantee continuous sample paths (continuous  $f(\mathbf{x} + t, \omega)$  for any  $\mathbf{x} \in \mathbb{R}^D$  and  $\omega \in \Omega$ ).

### KERNELS AND SPECTRAL DENSITIES

- ▶  $k(\mathbf{x}, \mathbf{x}')$  is a **covariance function** (i.e. positive definite)  $\rightarrow$  the  $n \times n$  **Gram matrix**  $\mathbf{K} = (k(\mathbf{x}_i, \mathbf{x}_j))_{i,j=1,...,n}$  is a **covariance matrix**.
- ▶ Bochner's theorem: A complex valued function  $k(\cdot)$  on  $\mathbb{R}^D$  is the covariance function of a weakly stationary continuous complex-valued stochastic process on  $\mathbb{R}^D$  iff

$$k(\mathbf{t}) = \int_{\mathbb{R}^D} e^{2\pi i \mathbf{s} \cdot \mathbf{t}} S(\mathbf{s}) d\mathbf{s}$$

- ► S(s) is the spectral density. S(s) is the energy allocated to the complex exponential basis function  $e^{2\pi i s \cdot t}$  at frequency s.
- ► For real-valued processes, think of  $e^{2\pi i \mathbf{s} \cdot \mathbf{t}}$  as a multi-dimensional sine wave with frequency  $\mathbf{s}$  and amplitude  $S(\mathbf{s})$ .
- ► Spectral density ←⇒Covariance function of stationary process ←⇒Smoothness properties of the process.

## COMMONLY USED COVARIANCE KERNELS

- ▶ Let r = ||x x'||. All kernels can be scaled by  $\sigma_f > 0$ .
- ▶ Squared exponential (SE)  $(\ell > 0)$

$$K_{SE}(r) = \exp\left(-rac{r^2}{2\ell^2}
ight)$$

- ▶ Spectral density  $S(s) = (2\pi\ell^2)^{D/2} \exp\left(-2\pi^2\ell^2s^2\right)$ . Higher frequencies tail of like a Gaussian (i.e. quickly).
- ▶ Infinitely mean square differentiable. Very smooth.
- ▶ Matérn ( $\ell > 0$ ,  $\nu > 0$ )

$$\mathcal{K}_{ extit{Matern}}(r) = rac{2^{1-
u}}{\Gamma(
u)} \left(rac{\sqrt{2
u r}}{\ell}
ight)^
u \mathcal{K}_
u \left(rac{\sqrt{2
u r}}{\ell}
ight)$$

- Spectral density behaves like a student-t density with  $2\nu$  degrees of freedom. For  $\nu=1/2$ , S(s) is Cauchy. Much weight on high frequency. Very rough.
- ▶  $\nu=3/2$  and  $\nu=5/2$  most useful for ML. As  $\nu\to\infty$ , Matérn's kernel approaches SE kernel.

# COMMONLY USED COVARIANCE KERNELS, CONT.

ightharpoonup  $\gamma$ -exponential ( $\ell > 0$ ,  $0 < \gamma \le 2$ )

$$K_{\gamma}(r) = \exp\left[-\left(\frac{r}{\ell}\right)^{\gamma}\right]$$

- Mean square differentiable only when  $\gamma=2$  (SE).
- ▶ Rational quadratic ( $\ell > 0$ ,  $\alpha > 0$ )

$$K_{RQ}(r) = \left(1 + \frac{r^2}{2\alpha\ell^2}\right)^{-\alpha}$$

- ► Scale mixture of SE covariance functions with different length-scales.
- $K_{RQ}(r)$  approaches the SE kernel as  $\alpha \to \infty$ .
- ▶  $k(r) = \int \exp(-r^2/2\ell^2) p(\ell) d\ell$  is the most general representation of an isotropic kernel with a valid covariance function in all dimensions D.

## MORE ON KERNELS

- Anisotropic version of isotropic kernels by setting  $r^2(\mathbf{x}, \mathbf{x}') = (\mathbf{x} \mathbf{x}')^T \mathbf{M} (\mathbf{x} \mathbf{x}')$  where **M** is positive definite.
- ▶ Automatic Relevance Determination (ARD):  $\mathbf{M} = Diag(\ell_1^{-2}, ..., \ell_D^{-2})$  is diagonal with different length scales.
- ► Factor kernels:  $M = \Lambda \Lambda^T + \Psi$ , where  $\Lambda$  is  $D \times k$  for low rank k.
- Length-scales  $\ell(x)$  that vary with x. Non-trivial to make positive definite, but see Gibbs kernel in Eq. 4.32.
- ► Kernels are often combined into **composite kernels**. Sum of kernels is a kernel. Product of kernels is a kernel.
- ► Kernels can be used for non-vectorial inputs by defining distance function between objects (e.g. words). String kernels for text analysis. Fisher kernels.

#### BAYESIAN INFERENCE FOR HYPERPARAMETERS

lacktriangle Kernel depends on hyperparameters heta. Example SE kernel  $[ heta=(\sigma_{\!f},\ell)^T]$ 

$$K(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2}\left(\frac{x - x'}{\ell}\right)^2\right)$$

▶ If the hyperparameters are unknown, just compute the posterior

$$p(\theta|\mathbf{y}, \mathbf{X}) \propto p(\mathbf{y}|\mathbf{X}, \theta)p(\theta|\mathbf{X}).$$

► We need to compute

$$p(\mathbf{y}|\mathbf{X},\theta) = \int p(\mathbf{y}|\mathbf{X},\mathbf{f},\theta)p(\mathbf{f}|\mathbf{X},\theta)d\mathbf{f}$$

where  $\mathbf{f} = f(\mathbf{X})$  is a vector with function values in the training data.

► For Gaussian process regression we can actually do this analytically

$$\log p(\mathbf{y}|\mathbf{X}, \theta) = -\frac{1}{2}\mathbf{f}^{\mathsf{T}}K^{-1}\mathbf{f} - \frac{1}{2}\log |K + \sigma_n^2I| - \frac{n}{2}\log(2\pi)$$

▶ RW takes a short-cut and estimates  $\theta$  by maximizing  $\log p(\mathbf{y}|\mathbf{X}, \theta)$ .

## Canadian wages - LML determination of $\ell$

