Multioutput Gaussian Processes

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GPRS
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Outline

Kalman Filter

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Kalman Filter

Simple Markov Chain

- Assume 1-d latent state, a vector over time, $\mathbf{x} = [x_1 \dots x_T]$.
- Markov property,

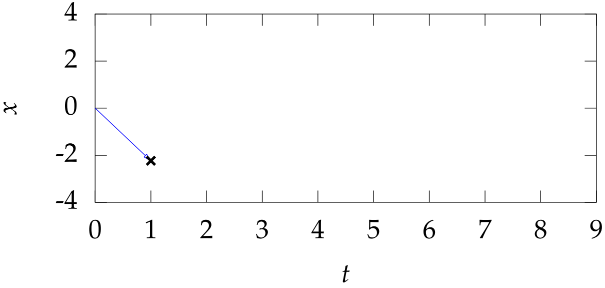
$$\begin{aligned} x_i =& x_{i-1} + \epsilon_i, \\ \epsilon_i \sim& \mathcal{N}(0, \alpha) \\ \implies x_i \sim& \mathcal{N}(x_{i-1}, \alpha) \end{aligned}$$

- Initial state,

$$x_0 \sim \mathcal{N}(0, \alpha_0)$$

- If $x_0 \sim \mathcal{N}(0, \alpha)$ we have a Markov chain for the latent states.
- Markov chain it is specified by an initial distribution (Gaussian) and a transition distribution (Gaussian).

Gauss Markov Chain

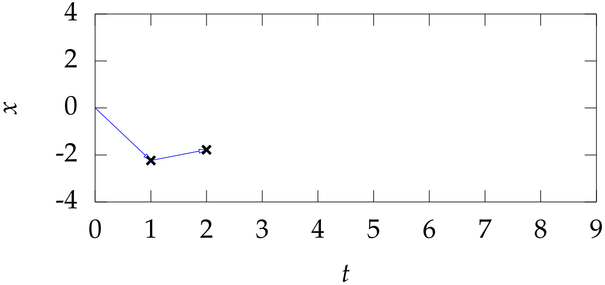


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_0 = 0.000, \quad \epsilon_1 = -2.24$$

$$x_1 = 0.000 - 2.24 = -2.24$$

Gauss Markov Chain

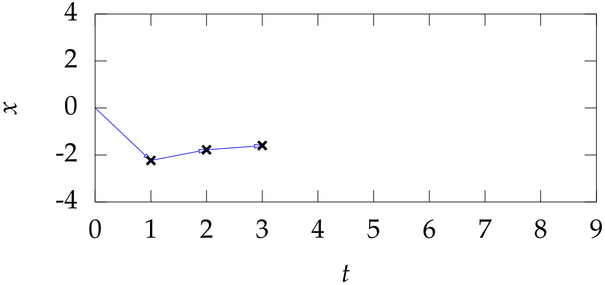


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_1 = -2.24, \quad \epsilon_2 = 0.457$$

$$x_2 = -2.24 + 0.457 = -1.78$$

Gauss Markov Chain

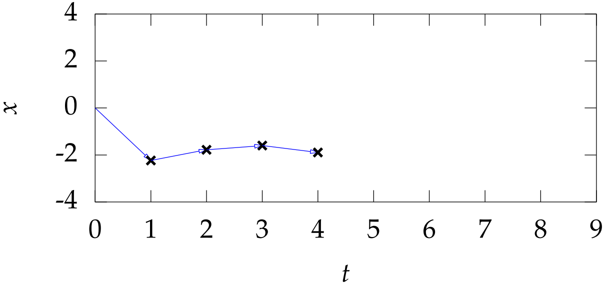


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_2 = -1.78, \quad \epsilon_3 = 0.178$$

$$x_3 = -1.78 + 0.178 = -1.6$$

Gauss Markov Chain

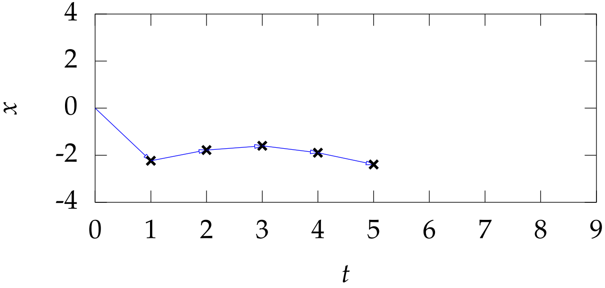


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_3 = -1.6, \quad \epsilon_4 = -0.292$$

$$x_4 = -1.6 - 0.292 = -1.89$$

Gauss Markov Chain

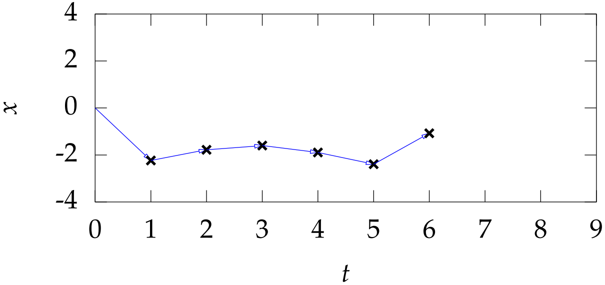


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_4 = -1.89, \quad \epsilon_5 = -0.501$$

$$x_5 = -1.89 - 0.501 = -2.39$$

Gauss Markov Chain

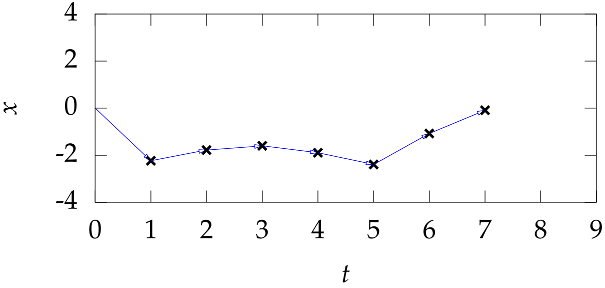


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_5 = -2.39, \quad \epsilon_6 = 1.32$$

$$x_6 = -2.39 + 1.32 = -1.08$$

Gauss Markov Chain

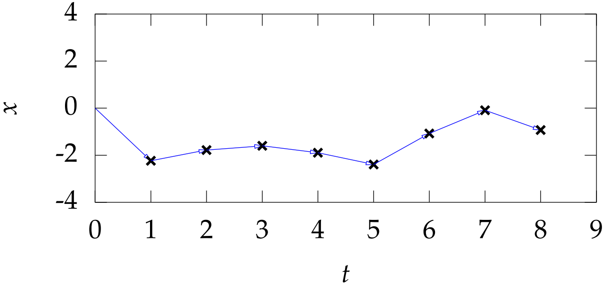


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_6 = -1.08, \quad \epsilon_7 = 0.989$$

$$x_7 = -1.08 + 0.989 = -0.0881$$

Gauss Markov Chain

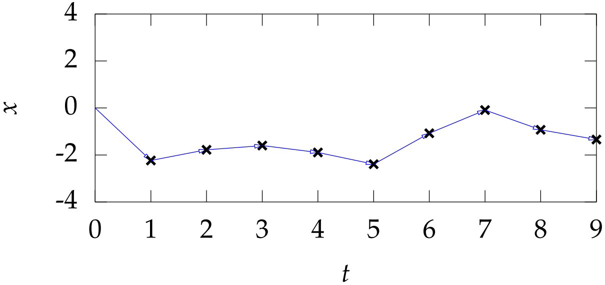


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_7 = -0.0881, \quad \epsilon_8 = -0.842$$

$$x_8 = -0.0881 - 0.842 = -0.93$$

Gauss Markov Chain



$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

$$x_8 = -0.93, \quad \epsilon_9 = -0.41$$

$$x_9 = -0.93 - 0.410 = -1.34$$

Multivariate Gaussian Properties: Reminder

If

$$\mathbf{z} \sim \mathcal{N}\left(\boldsymbol{\mu}, \mathbf{C}\right)$$

and

$$\mathbf{x} = \mathbf{W}\mathbf{z} + \mathbf{b}$$

then

$$\mathbf{x} \sim \mathcal{N}\left(\mathbf{W}\boldsymbol{\mu} + \mathbf{b}, \mathbf{W}\mathbf{C}\mathbf{W}^\top\right)$$

Multivariate Gaussian Properties: Reminder

Simplified: If

$$\mathbf{z} \sim \mathcal{N}\left(0, \sigma^2\mathbf{I}\right)$$

and

$$\mathbf{x} = \mathbf{W}\mathbf{z}$$

then

$$\mathbf{x} \sim \mathcal{N}\left(0, \sigma^2\mathbf{W}\mathbf{W}^\top\right)$$

Matrix Representation of Latent Variables

$$\begin{bmatrix} \boxed{x_1} \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$

$$x_1 = \epsilon_1$$

Matrix Representation of Latent Variables

$$\begin{bmatrix} x_1 \\ \boxed{x_2} \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$

$$x_2 = \epsilon_1 + \epsilon_2$$

Matrix Representation of Latent Variables

$$\begin{bmatrix} x_1 \\ x_2 \\ \boxed{x_3} \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$

$$x_3 = \epsilon_1 + \epsilon_2 + \epsilon_3$$

Matrix Representation of Latent Variables

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \boxed{x_4} \\ x_5 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$

$$x_4 = \epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4$$

Matrix Representation of Latent Variables

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \boxed{x_5} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ \boxed{1} & \boxed{1} & \boxed{1} & \boxed{1} & \boxed{1} \end{bmatrix} \times \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$

$$x_5 = \epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4 + \epsilon_5$$

Matrix Representation of Latent Variables

$$\mathbf{x} \quad = \quad \mathbf{L}_1 \quad \times \quad \epsilon$$

Multivariate Process

- Since $\mathbf{x}$ is linearly related to $\boldsymbol{\epsilon}$ we know $\mathbf{x}$ is a Gaussian process.
- Trick: we only need to compute the mean and covariance of $\mathbf{x}$ to determine that Gaussian.

Latent Process Mean

$$\mathbf{x} = \mathbf{L}_1\boldsymbol{\epsilon}$$

Latent Process Mean

$$\langle \mathbf{x} \rangle = \langle \mathbf{L}_1 \epsilon \rangle$$

Latent Process Mean

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Latent Process Mean

$$\langle \mathbf{x} \rangle = \mathbf{L}_1 \langle \boldsymbol{\epsilon} \rangle$$

$$\boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \alpha \mathbf{I}\right)$$

Latent Process Mean

$$\langle \mathbf{x} \rangle = \mathbf{L}_1 \mathbf{0}$$

Latent Process Mean

$$\langle \mathbf{x} \rangle = \mathbf{0}$$

Latent Process Covariance

$$\mathbf{x}\mathbf{x}^\top = \mathbf{L_1}\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top\mathbf{L_1}^\top$$

$$\mathbf{x}^\top = \boldsymbol{\epsilon}^\top\mathbf{L}^\top$$

Latent Process Covariance

$$\langle \mathbf{x}\mathbf{x}^\top \rangle = \left\langle \mathbf{L_1} \boldsymbol{\epsilon} \boldsymbol{\epsilon}^\top \mathbf{L_1}^\top \right\rangle$$

Latent Process Covariance

$$\left\langle \mathbf{x}\mathbf{x}^\top \right\rangle = \mathbf{L_1} \left\langle \boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top \right\rangle \mathbf{L_1}^\top$$

Latent Process Covariance

$$\langle \mathbf{x}\mathbf{x}^\top \rangle = \mathbf{L_1} \langle \boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top \rangle \mathbf{L_1}^\top$$

$$\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \alpha \mathbf{I})$$

Latent Process Covariance

$$\langle \mathbf{x}\mathbf{x}^\top \rangle = \alpha \mathbf{L}_\mathbf{1} \mathbf{L}_\mathbf{1}^\top$$

Latent Process

$$\mathbf{x} = \mathbf{L}_1 \boldsymbol{\epsilon}$$

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$$\Longrightarrow$$

Latent Process

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$$\Longrightarrow$$

$$\mathbf{x} \sim \mathcal{N}\left(\mathbf{0}, \alpha\mathbf{L_1}\mathbf{L_1}^\top\right)$$

Covariance for Latent Process II

- Make the variance dependent on time interval.
- Assume variance grows *linearly* with time.
- Justification: sum of two Gaussian distributed random variables is distributed as Gaussian with sum of variances.
- If variable's movement is additive over time (as described) variance scales linearly with time.

Covariance for Latent Process II

- Given
$$\boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \alpha \mathbf{I}\right) \Longrightarrow \boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \alpha \mathbf{L_1} \mathbf{L_1}^\top\right).$$
Then
$$\boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \Delta t \alpha \mathbf{I}\right) \Longrightarrow \boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \Delta t \alpha \mathbf{L_1} \mathbf{L_1}^\top\right).$$
where Δt is the time interval between observations.

Covariance for Latent Process II

$$\boldsymbol{\epsilon} \sim \mathcal{N}\left(0, \alpha \Delta t \mathbf{I}\right), \quad \mathbf{x} \sim \mathcal{N}\left(0, \alpha \Delta t \mathbf{L_1} \mathbf{L_1}^\top\right)$$

Covariance for Latent Process II

$$\boldsymbol{\epsilon} \sim \mathcal{N}\left(0, \alpha \Delta t \mathbf{I}\right), \quad \mathbf{x} \sim \mathcal{N}\left(0, \alpha \Delta t \mathbf{L_1} \mathbf{L_1}^\top\right)$$

$$\mathbf{K} = \alpha \Delta t \mathbf{L_1} \mathbf{L_1}^\top$$

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$$\mathbf{K} = \alpha\Delta t\mathbf{L_1}\mathbf{L_1}^\top$$

$$k_{i,j} = \alpha\Delta t\mathbf{l}_{:,i}^\top\mathbf{l}_{:,j}$$

where $\mathbf{l}_{:,k}$ is a vector from the kth row of $\mathbf{L_1}$: the first k elements are one, the next $T - k$ are zero.

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$$k_{i,j} = \alpha\Delta t \min(i, j)$$

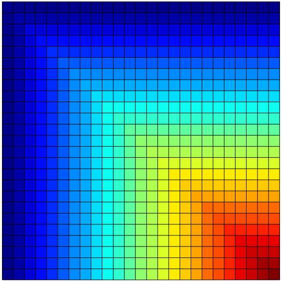
define $\Delta t i = t_i$ so

$$k_{i,j} = \alpha \min(t_i, t_j) = k(t_i, t_j)$$

Markov Process

$$k(t, t') = \alpha \min(t, t')$$

- Covariance matrix is built using the *inputs* to the function t.



Covariance Functions

Where did this covariance matrix come from?

Markov Process

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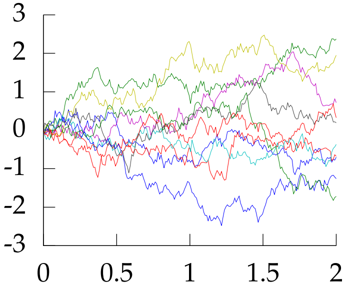
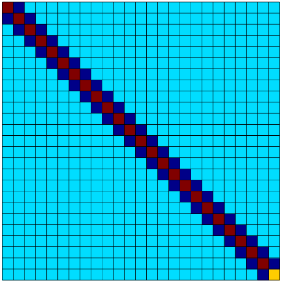


Markov Process

Visualization of inverse covariance (precision).

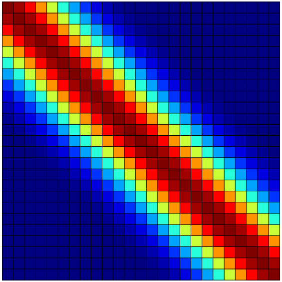
- Precision matrix is sparse: only neighbours in matrix are non-zero.
- This reflects *conditional* independencies in data.
- In this case *Markov* structure.



Exponentiated Quadratic Kernel Function (RBF, Squared Exponential, Gaussian)

$$k(\mathbf{x}, \mathbf{x}') = \alpha \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|_2^2}{2\ell^2}\right)$$

- Covariance matrix is built using the *inputs* to the function $\mathbf{x}$.
- For the example above it was based on Euclidean distance.
- The covariance function is also know as a kernel.



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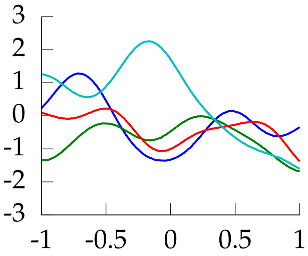


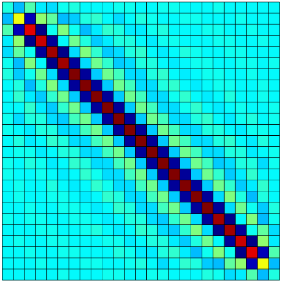
Covariance Functions

Where did this covariance matrix come from?

Exponentiated Quadratic

Visualization of inverse covariance (precision).

- Precision matrix is not sparse.
- Each point is dependent on all the others.
- In this case non-Markovian.



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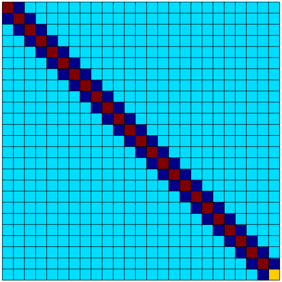


Simple Kalman Filter I

- We have state vector $\mathbf{X} = \left[\mathbf{x}_1 \ldots \mathbf{x}_q\right] \in \mathbb{R}^{T \times q}$ and if each state evolves independently we have

$$p(\mathbf{X}) = \prod_{i=1}^{q} p(\mathbf{x}_{:,i})$$
$$p(\mathbf{x}_{:,i}) = \mathcal{N}\left(\mathbf{x}_{:,i}|\mathbf{0}, \mathbf{K}\right).$$

- We want to obtain outputs through:

$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:}$$

Stacking and Kronecker Products I

- Represent with a 'stacked' system:

$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\mathbf{0}, \mathbf{I} \otimes \mathbf{K}\right)$$

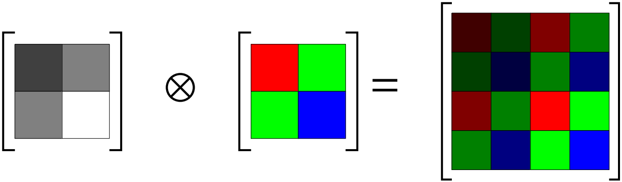
  where the stacking is placing each column of $\mathbf{X}$ one on top of another as

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_{:,1} \\ \mathbf{x}_{:,2} \\ \vdots \\ \mathbf{x}_{:,q} \end{bmatrix}$$

Kronecker Product

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \otimes \mathbf{K} = \begin{bmatrix} a\mathbf{K} & b\mathbf{K} \\ c\mathbf{K} & d\mathbf{K} \end{bmatrix}$$

Kronecker Product



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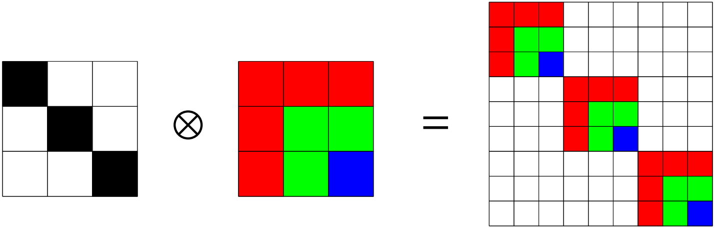
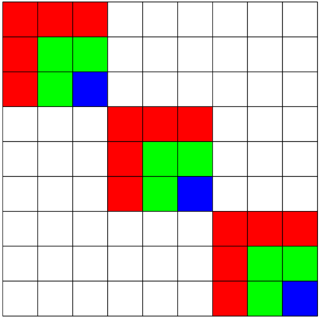
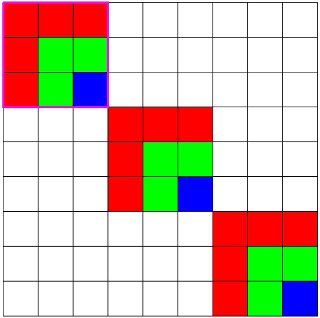
Column Stacking





For this stacking the marginal distribution over *time* is given by the block diagonals.



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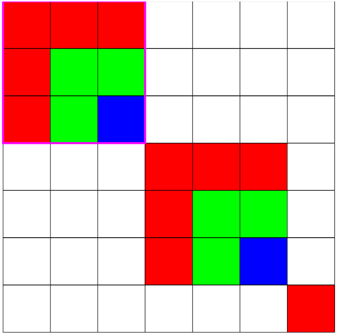

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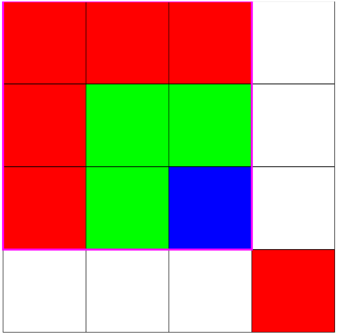

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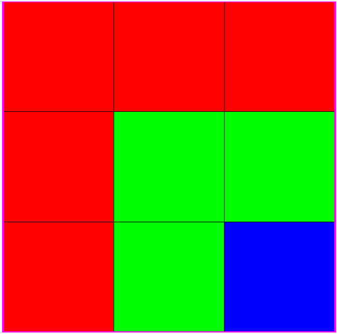


For this stacking the marginal distribution over *time* is given by the block diagonals.

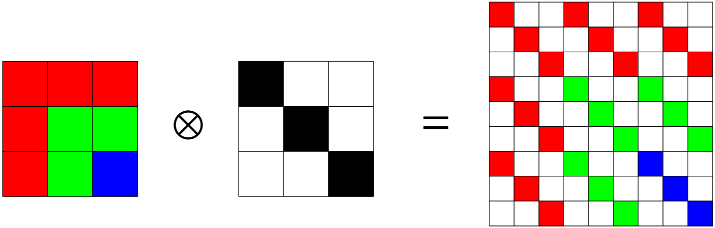
Two Ways of Stacking

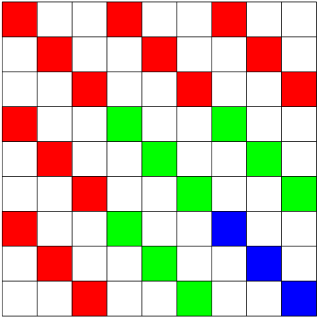
Can also stack each row of $\mathbf{X}$ to form column vector:

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_{1,:} \\ \mathbf{x}_{2,:} \\ \vdots \\ \mathbf{x}_{T,:} \end{bmatrix}$$

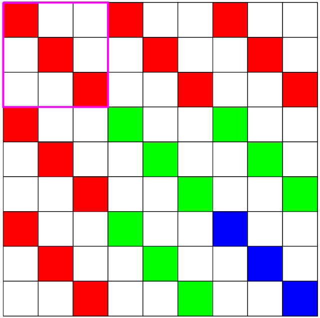
$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\mathbf{0}, \mathbf{K} \otimes \mathbf{I}\right)$$

Row Stacking





For this stacking the marginal distribution over the latent *dimensions* is given by the block diagonals.



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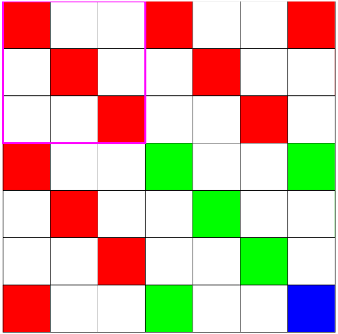

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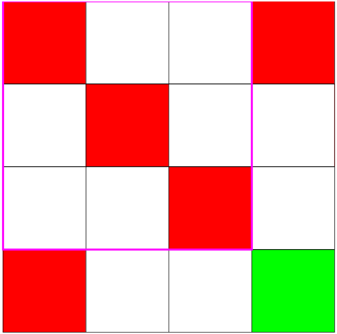

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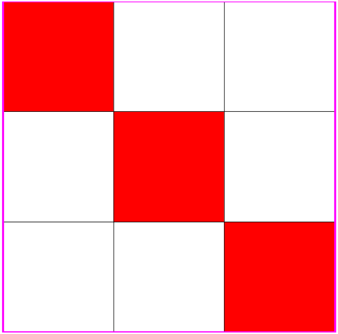

For this stacking the marginal distribution over the latent *dimensions* is given by the block diagonals.

Observed Process

The observations are related to the latent points by a linear mapping matrix,

$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:} + \boldsymbol{\epsilon}_{i,:}$$

$$\boldsymbol{\epsilon} \sim \mathcal{N}\left(0, \sigma^2\mathbf{I}\right)$$

Mapping from Latent Process to Observed

$$\begin{bmatrix} \mathbf{W} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{W} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{W} \end{bmatrix} \times \begin{bmatrix} \mathbf{x}_{1,:} \\ \mathbf{x}_{2,:} \\ \mathbf{x}_{3,:} \end{bmatrix} = \begin{bmatrix} \mathbf{W}\mathbf{x}_{1,:} \\ \mathbf{W}\mathbf{x}_{2,:} \\ \mathbf{W}\mathbf{x}_{3,:} \end{bmatrix}$$

Output Covariance

This leads to a covariance of the form

$$(\mathbf{I} \otimes \mathbf{W})(\mathbf{K} \otimes \mathbf{I})(\mathbf{I} \otimes \mathbf{W}^\top) + \mathbf{I}\sigma^2$$

Using $(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = \mathbf{AC} \otimes \mathbf{BD}$ This leads to

$$\mathbf{K} \otimes \mathbf{W}\mathbf{W}^\top + \mathbf{I}\sigma^2$$

or

$$\mathbf{y} \sim \mathcal{N}\left(0, \mathbf{W}\mathbf{W}^\top \otimes \mathbf{K} + \mathbf{I}\sigma^2\right)$$

Kernels for Vector Valued Outputs: A Review

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Kernels for Vector-Valued Functions: A Review

By Mauricio A. Álvarez,
Lorenzo Rosasco and Neil D. Lawrence

Kronecker Structure GPs

- This Kronecker structure leads to several published models.
$$(\mathbf{K}(\mathbf{x}, \mathbf{x}'))_{d,d'} = k(\mathbf{x}, \mathbf{x}')k_T(d, d'),$$
where k has $\mathbf{x}$ and k_T has n as inputs.
- Can think of multiple output covariance functions as covariances with augmented input.
- Alongside $\mathbf{x}$ we also input the d associated with the *output* of interest.

Separable Covariance Functions

- Taking $\mathbf{B} = \mathbf{W}\mathbf{W}^\top$ we have a matrix expression across outputs.
$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}')\mathbf{B},$$
where $\mathbf{B}$ is a $p \times p$ symmetric and positive semi-definite matrix.
- $\mathbf{B}$ is called the *coregionalization* matrix.
- We call this class of covariance functions *separable* due to their product structure.

Sum of Separable Covariance Functions

- In the same spirit a more general class of kernels is given by

$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{q} k_j(\mathbf{x}, \mathbf{x}')\mathbf{B}_j.$$

- This can also be written as

$$\mathbf{K}(\mathbf{X}, \mathbf{X}) = \sum_{j=1}^{q} \mathbf{B}_j \otimes k_j(\mathbf{X}, \mathbf{X}),$$

- This is like several Kalman filter-type models added together, but each one with a different set of latent functions.
- We call this class of kernels sum of separable kernels (SoS kernels).

Geostatistics

- Use of GPs in Geostatistics is called kriging.
- These multi-output GPs pioneered in geostatistics: prediction over vector-valued output data is known as *cokriging*.
- The model in geostatistics is known as the *linear model of coregionalization* (LMC, Journel and Huijbregts (1978); Goovaerts (1997)).
- Most machine learning multitask models can be placed in the context of the LMC model.

Weighted sum of Latent Functions

- In the linear model of coregionalization (LMC) outputs are expressed as linear combinations of independent random functions.
- In the LMC, each component f_d is expressed as a linear sum

$$f_d(\mathbf{x}) = \sum_{j=1}^{q} w_{d,j} u_j(\mathbf{x}).$$

  where the latent functions are independent and have covariance functions $k_j(\mathbf{x}, \mathbf{x}')$.
- The processes $\{f_j(\mathbf{x})\}_{j=1}^{q}$ are independent for $q \neq j'$.

Kalman Filter Special Case

- The Kalman filter is an example of the LMC where $u_i(\mathbf{x}) \rightarrow x_i(t)$.
- I.e. we've moved form time input to a more general input space.
- In matrix notation:
  1. Kalman filter
  $$\mathbf{F} = \mathbf{W}\mathbf{X}$$
  2. LMC
  $$\mathbf{F} = \mathbf{W}\mathbf{U}$$

  where the rows of these matrices $\mathbf{F}$, $\mathbf{X}$, $\mathbf{U}$ each contain q samples from their corresponding functions at a different time (Kalman filter) or spatial location (LMC).

Intrinsic Coregionalization Model

- If one covariance used for latent functions (like in Kalman filter).
- This is called the intrinsic coregionalization model (ICM, Goovaerts (1997)).
- The kernel matrix corresponding to a dataset $\mathbf{X}$ takes the form

$$\mathbf{K}(\mathbf{X}, \mathbf{X}) = \mathbf{B} \otimes k(\mathbf{X}, \mathbf{X}).$$

Autokrigeability

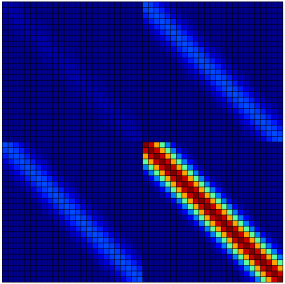
- If outputs are noise-free, maximum likelihood is equivalent to independent fits of $\mathbf{B}$ and $k(\mathbf{x}, \mathbf{x}')$ (Helterbrand and Cressie, 1994).
- In geostatistics this is known as autokrigeability (Wackernagel, 2003).
- In multitask learning its the cancellation of intertask transfer (Bonilla et al., 2008).

Intrinsic Coregionalization Model

$$\mathbf{K}(\mathbf{X},\mathbf{X}) = \mathbf{w}\mathbf{w}^\top \otimes k(\mathbf{X},\mathbf{X}).$$

$$\mathbf{w} = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 1 & 5 \\ 5 & 25 \end{bmatrix}$$



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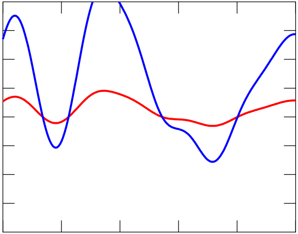

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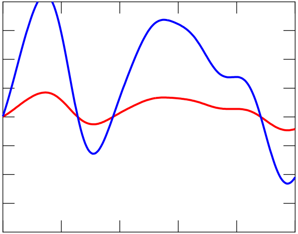

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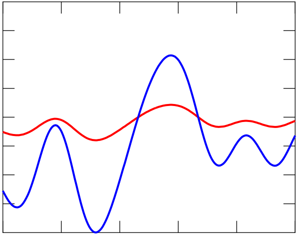

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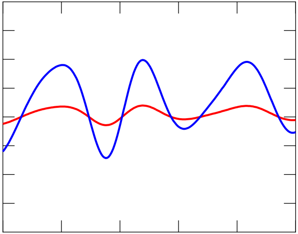

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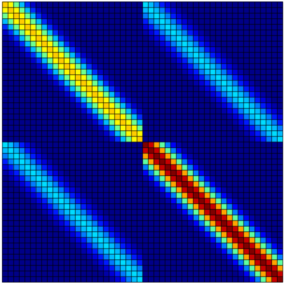

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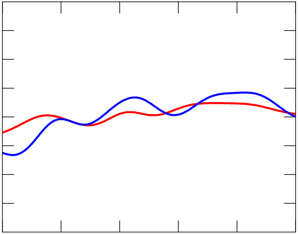

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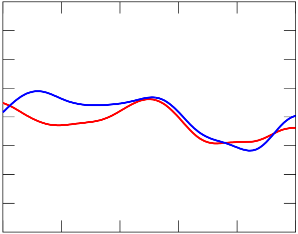

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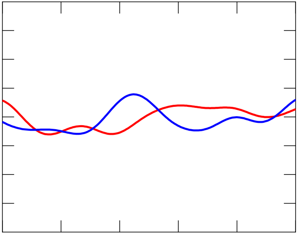

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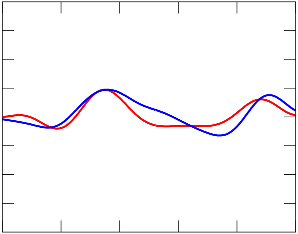


LMC Samples

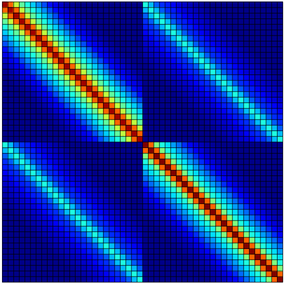
$$\mathbf{K}(\mathbf{X},\mathbf{X}) = \mathbf{B}_1 \otimes k_1(\mathbf{X},\mathbf{X}) + \mathbf{B}_2 \otimes k_2(\mathbf{X},\mathbf{X})$$

$$\mathbf{B}_1 = \begin{bmatrix} 1.4 & 0.5 \\ 0.5 & 1.2 \end{bmatrix}$$

$$\ell_1 = 1$$

$$\mathbf{B}_2 = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1.3 \end{bmatrix}$$

$$\ell_2 = 0.2$$



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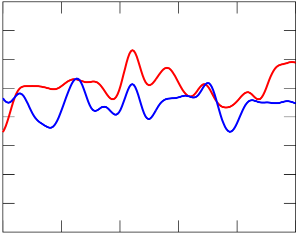

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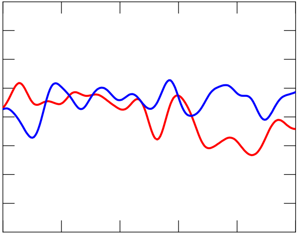

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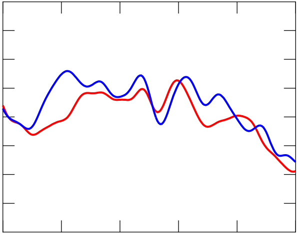

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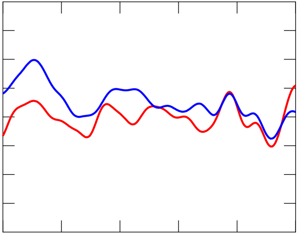

LMC in Machine Learning and Statistics

- Used in machine learning for GPs for multivariate regression and in statistics for computer emulation of expensive multivariate computer codes.
- Imposes the correlation of the outputs explicitly through the set of coregionalization matrices.
- Setting $\mathbf{B} = \mathbf{I}_p$ assumes outputs are conditionally independent given the parameters $\boldsymbol{\theta}$. (Minka and Picard, 1997; Lawrence and Platt, 2004; Yu et al., 2005).
- More recent approaches for multiple output modeling are different versions of the linear model of coregionalization.

Semiparametric Latent Factor Model

- Coregionalization matrices are rank 1 Teh et al. (2005). rewrite equation (**??**) as

$$\mathbf{K}(\mathbf{X},\mathbf{X}) = \sum_{j=1}^{q} \mathbf{w}_{:,j}\mathbf{w}_{:,j}^{\top} \otimes k_j(\mathbf{X},\mathbf{X}).$$

- Like the Kalman filter, but each latent function has a *different* covariance.
- Authors suggest using an exponentiated quadratic characteristic length-scale for each input dimension.

Semiparametric Latent Factor Model Samples

$$\mathbf{K}(\mathbf{X},\mathbf{X}) = \mathbf{w}_{:,1}\mathbf{w}_{:,1}^{\top} \otimes k_1(\mathbf{X},\mathbf{X}) + \mathbf{w}_{:,2}\mathbf{w}_{:,2}^{\top} \otimes k_2(\mathbf{X},\mathbf{X})$$

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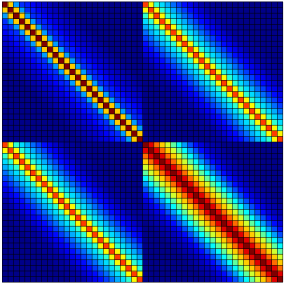

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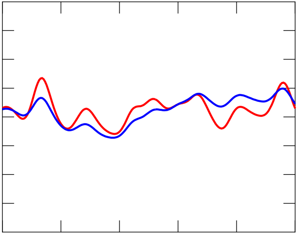

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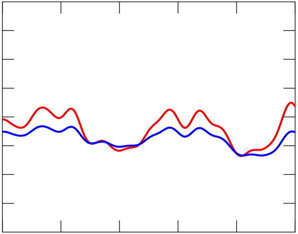

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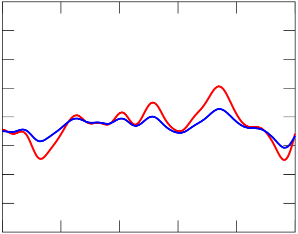

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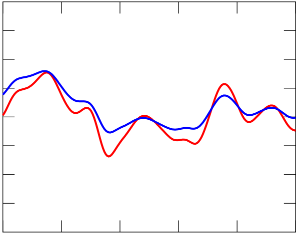

Gaussian processes for Multi-task, Multi-output and Multi-class

- Bonilla et al. (2008) suggest ICM for multitask learning.
- Use a PPCA form for $\mathbf{B}$: similar to our Kalman filter example.
- Refer to the autokrigeability effect as the cancellation of inter-task transfer.
- Also discuss the similarities between the multi-task GP and the ICM, and its relationship to the SLFM and the LMC.

Multitask Classification

- Mostly restricted to the case where the outputs are conditionally independent given the hyperparameters ϕ (Minka and Picard, 1997; Williams and Barber, 1998; Lawrence and Platt, 2004; Seeger and Jordan, 2004; Yu et al., 2005; Rasmussen and Williams, 2006).
- Intrinsic coregionalization model has been used in the multiclass scenario. Skolidis and Sanguinetti (2011) use the intrinsic coregionalization model for classification, by introducing a probit noise model as the likelihood.
- Posterior distribution is no longer analytically tractable: approximate inference is required.

Computer Emulation

- A statistical model used as a surrogate for a computationally expensive computer model.
- Higdon et al. (2008) use the linear model of coregionalization to model images representing the evolution of the implosion of steel cylinders.
- In Conti and O'Hagan (2009) use the ICM to model a vegetation model: called the Sheffield Dynamic Global Vegetation Model (Woodward et al., 1998).

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