Multioutput, Multitask and Mechanistic

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CVPR
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Outline

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Simple Markov Chain

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

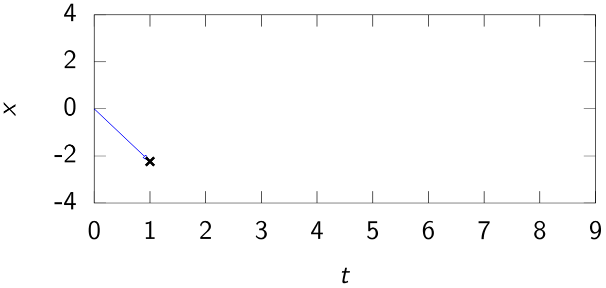
$$\begin{aligned} x_i =& x_{i-1} + \epsilon_i, \\ \epsilon_i \sim& \mathcal{N}(0, \alpha) \\ \implies x_i \sim& \mathcal{N}(x_{i-1}, \alpha) \end{aligned}$$

- 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

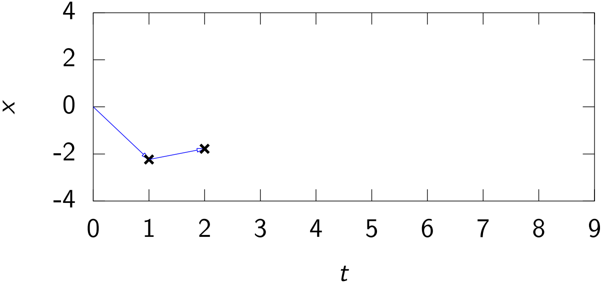


$$x_0 = 0, \quad \boldsymbol{\epsilon}_i \sim \mathcal{N}(0, 1)$$

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

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

Gauss Markov Chain

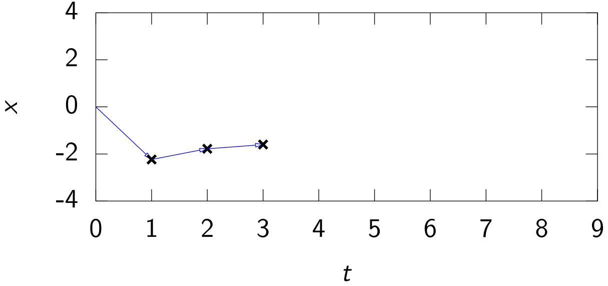


$$x_0 = 0, \quad \boldsymbol{\epsilon}_i \sim \mathcal{N}(0, 1)$$

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

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

Gauss Markov Chain

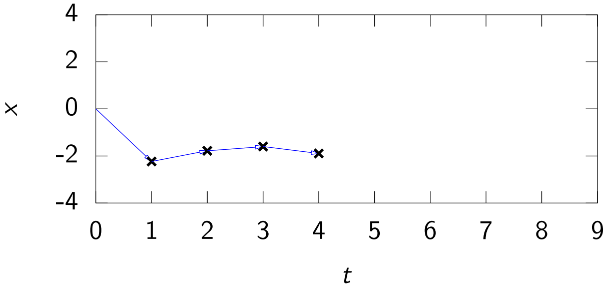


$$x_0 = 0, \quad \boldsymbol{\epsilon}_i \sim \mathcal{N}(0, 1)$$

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

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

Gauss Markov Chain

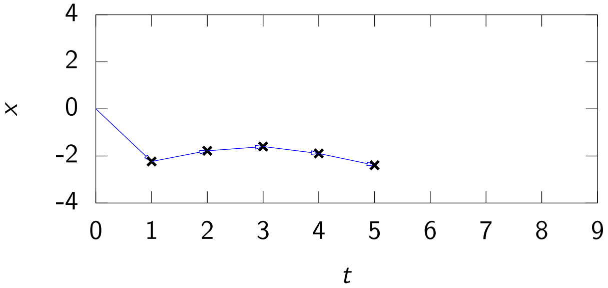


$$x_0 = 0, \quad \boldsymbol{\epsilon}_i \sim \mathcal{N}(0, 1)$$

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

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

Gauss Markov Chain

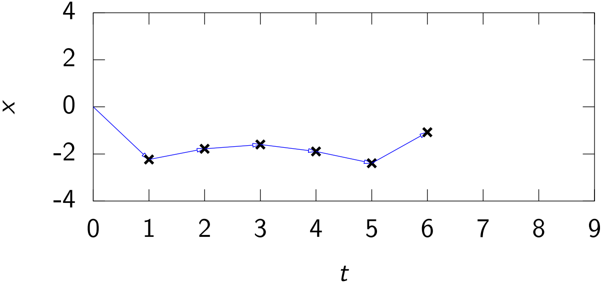


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

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

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

Gauss Markov Chain

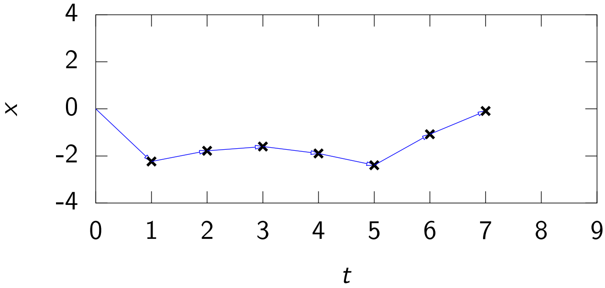


$$x_0 = 0, \quad \boldsymbol{\epsilon}_i \sim \mathcal{N}(0, 1)$$

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

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

Gauss Markov Chain

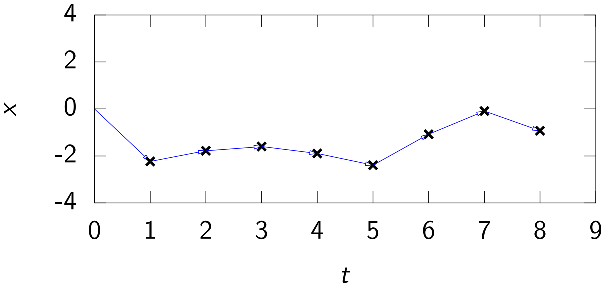


$$x_0 = 0, \quad \epsilon_i \sim \mathcal{N}(0, 1)$$

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

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

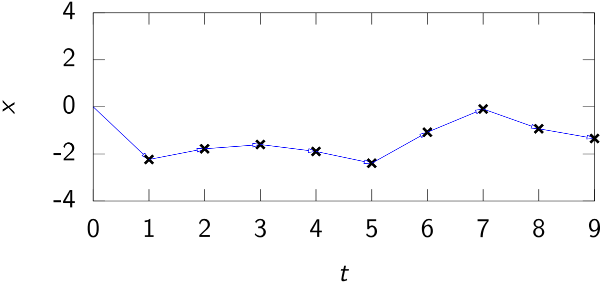
Gauss Markov Chain



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

$$x_7 = -0.0881, \quad \epsilon_8 = -0.842$$
$$x_8 = -0.0881 - 0.842 = -0.93$$

Gauss Markov Chain



$$x_0 = 0, \quad \boldsymbol{\epsilon}_i \sim \mathcal{N}(0, 1)$$

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

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

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

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

$$x_1 = \epsilon_1$$

Matrix Representation of Latent Variables

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

$$x_2 = \epsilon_1 + \epsilon_2$$

Matrix Representation of Latent Variables

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

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

Matrix Representation of Latent Variables

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

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

Matrix Representation of Latent Variables

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

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

Matrix Representation of Latent Variables

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

Multivariate Process

- Since $\mathbf{x}$ is linearly related to ϵ 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

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

Latent Process Mean

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

Latent Process Mean

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Latent Process Mean

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

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

Latent Process Mean

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

Latent Process Mean

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

Latent Process Covariance

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

Latent Process Covariance

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

Latent Process Covariance

$$\left\langle \mathbf{x}\mathbf{x}^{\top} \right\rangle = \mathbf{L}_1 \left\langle \epsilon\epsilon^{\top} \right\rangle \mathbf{L}_1^{\top}$$

Latent Process Covariance

$$\left\langle \mathbf{x}\mathbf{x}^{\top} \right\rangle = \mathbf{L}_1 \left\langle \boldsymbol{\epsilon}\boldsymbol{\epsilon}^{\top} \right\rangle \mathbf{L}_1^{\top}$$

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

Latent Process Covariance

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

Latent Process

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

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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

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

Covariance for Latent Process II

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

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

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

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.

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

define $\Delta t i = t_i$ so

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

Covariance for Latent Process II

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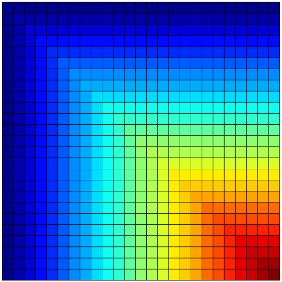
Covariance Functions

Where did this covariance matrix come from?

Markov Process

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

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



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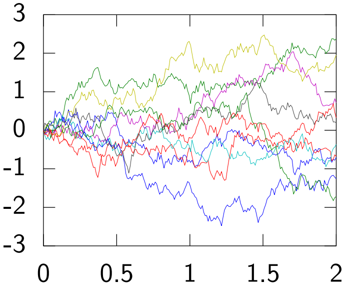


Simple Kalman Filter I

- We have state vector $\mathbf{X} = [\mathbf{x}_1 \dots \mathbf{x}_q] \in \mathbb{R}^{T \times q}$ and if each state evolves independently we have
- $p(\mathbf{X}) = \prod_{i=1}^{q} p(\mathbf{x}_{:,i})\ p(\mathbf{x}_{:,i}) = \mathcal{N}(\mathbf{x}_{:,i}|\mathbf{0}, \mathbf{K})$.
- We want to obtain outputs through:

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

Stacking and Kronecker Products I

- Represent with a 'stacked' system:

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

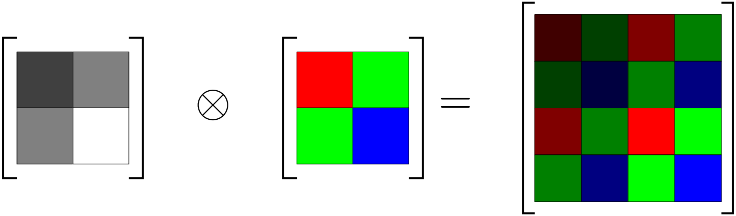
where the stacking is placing each column of $\mathbf{X}$ one on top of another as

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

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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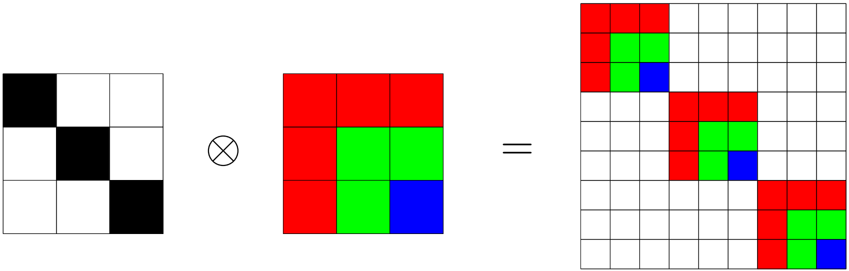
Column Stacking



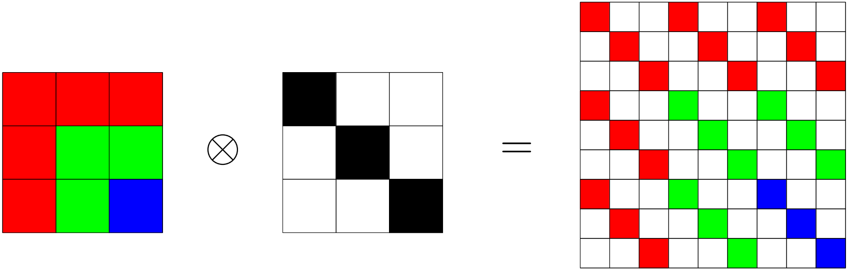
Two Ways of Stacking

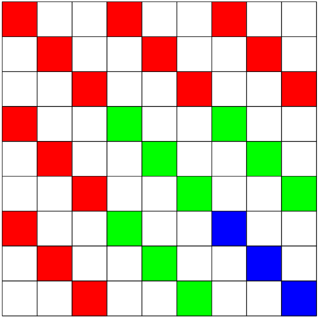
Can also stack as follows:

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

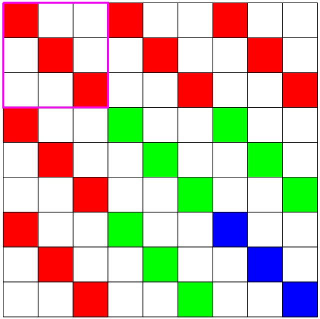
$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\mathbf{0}, \mathbf{K} \otimes \mathbf{I}\right)$$

Row Stacking





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



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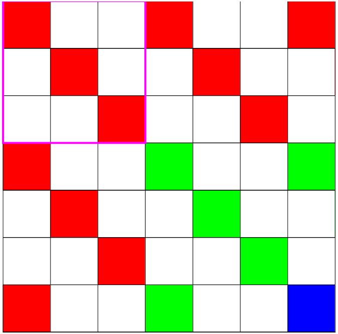

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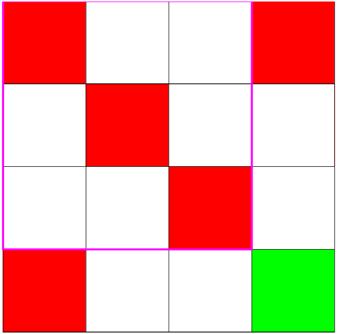

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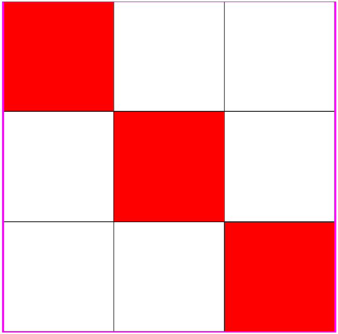


For this stacking the marginal distribution over the latent variables is given by the block diagonals.

Observed Process

If we relate the observations to the data as follows:

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

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

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

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

or

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

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, **??**).
- 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 $u_i(\mathbf{x}) \to x_i(t)$.
- 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, **?**).
- 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

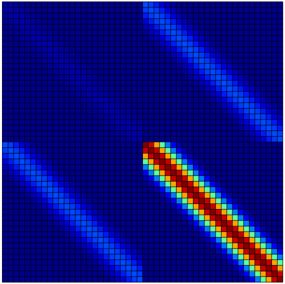
- If outputs are noise-free, maximum likelihood is equivalent to independent fits of $\mathbf{B}$ and $k(\mathbf{x}, \mathbf{x}')$ (**?**).
- In geostatistics this is known as autokrigeability (**?**).
- In multitask learning its the cancellation of intertask transfer (**?**).

Intrinsic Coregionalization Model

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

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

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



Intrinsic Coregionalization Model

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

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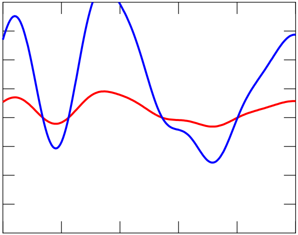

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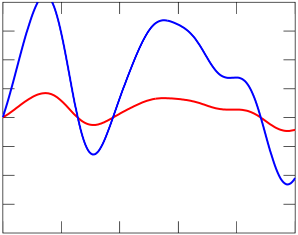

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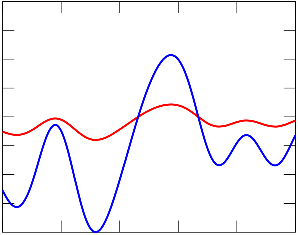

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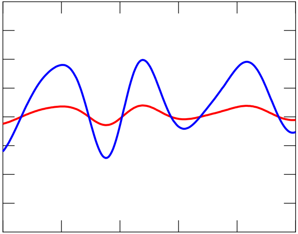

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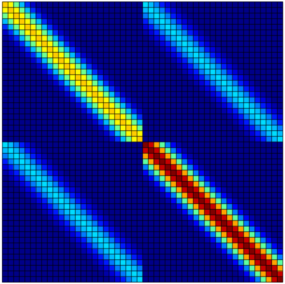

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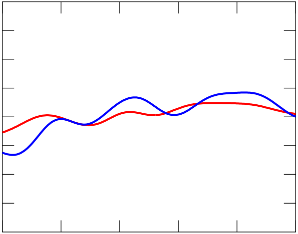

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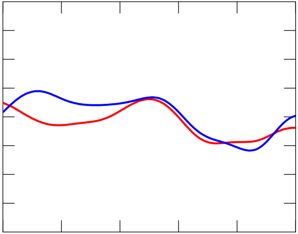

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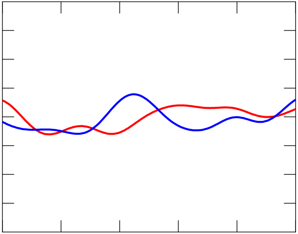

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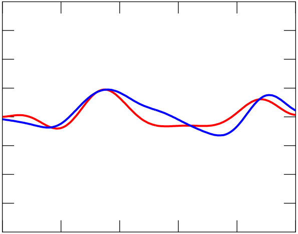


LMC Samples

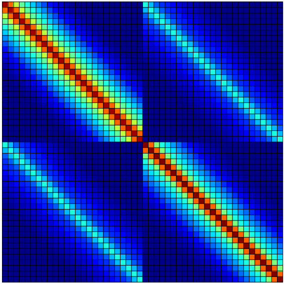
$$\mathbf{K}(\mathbf{X}, \mathbf{X}) = \mathbf{B}_1 \otimes k_1(\mathbf{X}, \mathbf{X}) + \mathbf{B}_2 \otimes k_2(\mathbf{X}, \mathbf{X})$$

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

$$\ell_1 = 1$$

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

$$\ell_2 = 0.2$$



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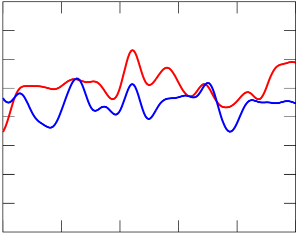

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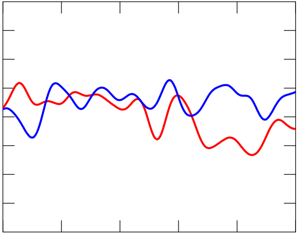

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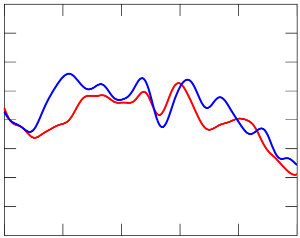

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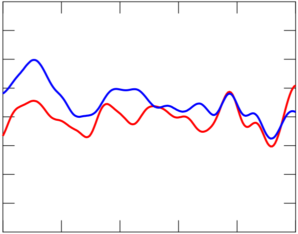

LMC in Machine Learning and Statistics

- 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 $\boldsymbol{\theta}$. (**???**).
- 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 **?**. 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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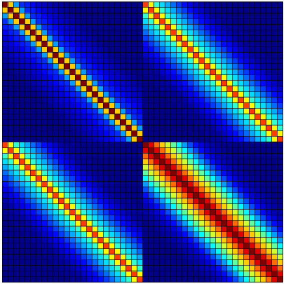

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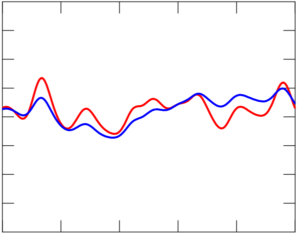

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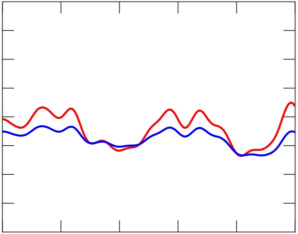

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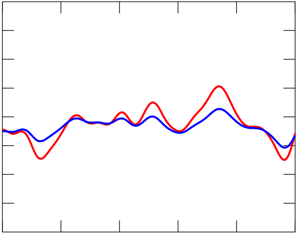

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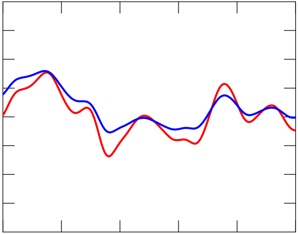


Gaussian processes for Multi-task, Multi-output and Multi-class

- **?** suggest ICM for multitask learning.
- Use a PPCA form for **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 (**??????**).
- Intrinsic coregionalization model has been used in the multiclass scenario. **?** 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.
- **?** use the linear model of coregionalization to model images representing the evolution of the implosion of steel cylinders.
- In **?** use the ICM to model a vegetation model: called the Sheffield Dynamic Global Vegetation Model (**?**).

Outline

Convolution Process

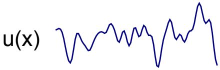
- A convolution process is a moving-average construction that guarantees a valid covariance function.
- Consider a set of functions $\{f_j(\mathbf{x})\}_{j=1}^{p}$.
- Each function can be expressed as

$$f_j(\mathbf{x}) = \int_{\mathcal{X}} G_j(\mathbf{x} - \mathbf{z})u(\mathbf{z})\mathrm{d}\mathbf{z} = G_j(\mathbf{x}) * u(\mathbf{x}).$$

- Influence of more than one latent function, $\{u_i(\mathbf{z})\}_{i=1}^{q}$ and inclusion of an independent process $w_j(\mathbf{x})$

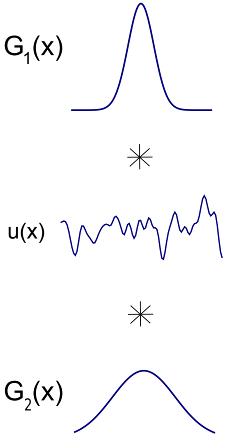
$$y_j(\mathbf{x}) = f_j(\mathbf{x}) + w_j(\mathbf{x}) = \sum_{i=1}^{q} \int_{\mathcal{X}} G_{j,i}(\mathbf{x} - \mathbf{z})u_i(\mathbf{z})\mathrm{d}\mathbf{z} + w_j(\mathbf{x}).$$

A pictorial representation



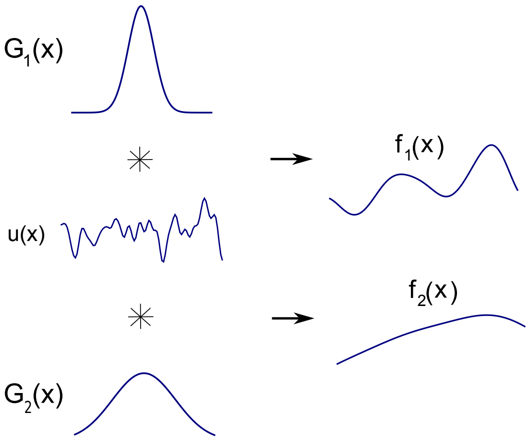
u(x): latent function.

A pictorial representation



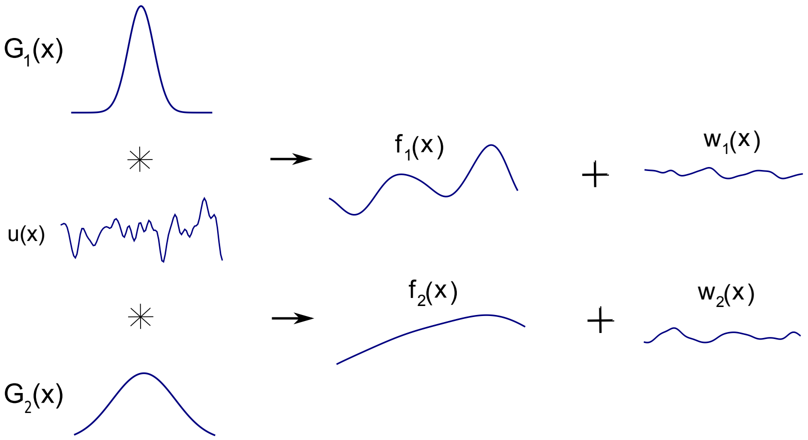
u(x): latent function.
G(x): smoothing kernel.

A pictorial representation



u(x): latent function.
G(x): smoothing kernel.
f(x): output function.

A pictorial representation



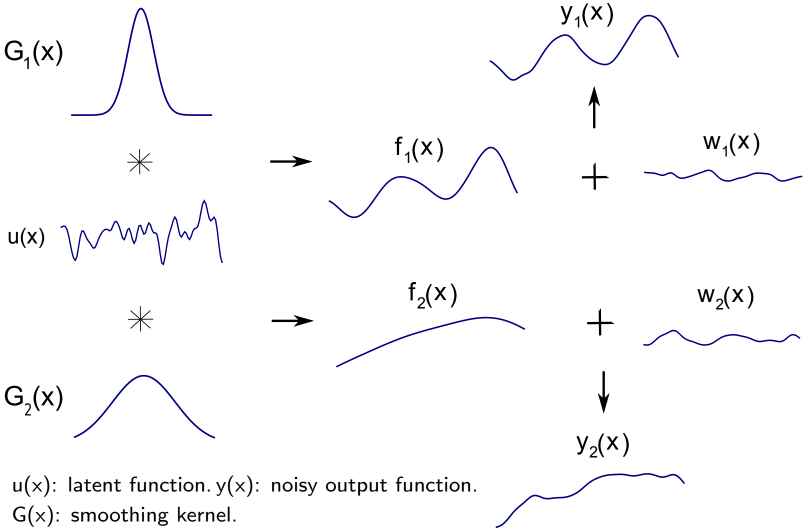
u(x): latent function.

G(x): smoothing kernel.

f(x): output function.

w(x): independent process.

A pictorial representation



u(x): latent function. y(x): noisy output function.

G(x): smoothing kernel.

f(x): output function.

w(x): independent process.

Covariance of the output functions.

The covariance between $y_j(\mathbf{x})$ and $y_{j'}(\mathbf{x}')$ is given as

$$\text{cov}\left[y_j(\mathbf{x}), y_{j'}(\mathbf{x}')\right] = \text{cov}\left[f_j(\mathbf{x}), f_{j'}(\mathbf{x}')\right] + \text{cov}\left[w_j(\mathbf{x}), w_{j'}(\mathbf{x}')\right]\delta_{j,j'}$$

where

$$\text{cov}\left[f_j(\mathbf{x}), f_{j'}(\mathbf{x}')\right] = \int_{\mathcal{X}} G_j(\mathbf{x}-\mathbf{z}) \int_{\mathcal{X}} G_{j'}(\mathbf{x}'-\mathbf{z}')\text{cov}\left[u(\mathbf{z}), u(\mathbf{z}')\right] \mathrm{d}\mathbf{z}'\mathrm{d}\mathbf{z}$$

Different forms of covariance for the output functions.

- Input *Gaussian process*

$$\mathrm{cov}\left[f_j, f_{j'}\right] = \int_{\mathcal{X}} G_j(\mathbf{x}-\mathbf{z}) \int_{\mathcal{X}} G_{j'}(\mathbf{x}'-\mathbf{z}') k_{u,u}(\mathbf{z},\mathbf{z}') \mathrm{d}\mathbf{z}' \mathrm{d}\mathbf{z}$$

- Input *white noise process*

$$\mathrm{cov}\left[f_j, f_{j'}\right] = \int_{\mathcal{X}} G_j(\mathbf{x}-\mathbf{z}) G_{j'}(\mathbf{x}'-\mathbf{z}) \mathrm{d}\mathbf{z}$$

- Covariance between output functions and latent functions

$$\mathrm{cov}\left[f_j, u\right] = \int_{\mathcal{X}} G_j(\mathbf{x}-\mathbf{z}') k_{u,u}(\mathbf{z}',\mathbf{z}) \mathrm{d}\mathbf{z}'$$

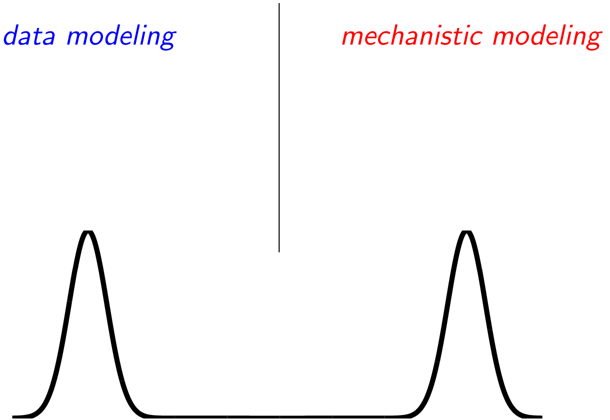
Styles of Machine Learning

Background: interpolation is easy, extrapolation is hard

- Urs Hölzle keynote talk at NIPS 2005.
  - Emphasis on massive data sets.
  - Let the data do the work—more data, less extrapolation.
- Alternative paradigm:
  - Very scarce data: computational biology, human motion.
  - How to generalize from scarce data?
  - Need to include more assumptions about the data (e.g. invariances).

General Approach

Broadly Speaking: Two approaches to modeling



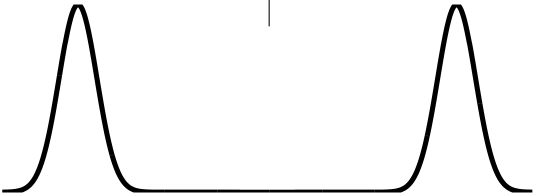
General Approach

Broadly Speaking: Two approaches to modeling

data modeling

let the data "speak"

mechanistic modeling



General Approach

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data modeling

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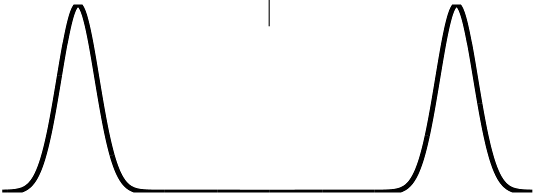
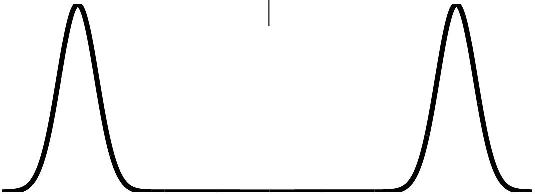
impose physical laws



General Approach

Broadly Speaking: Two approaches to modeling

data modeling	*mechanistic modeling*
let the data "speak"	impose physical laws
data driven	



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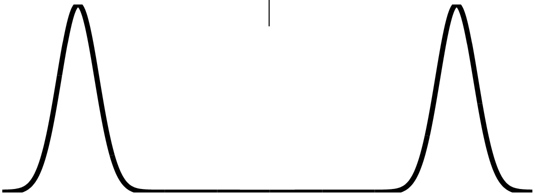

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Broadly Speaking: Two approaches to modeling

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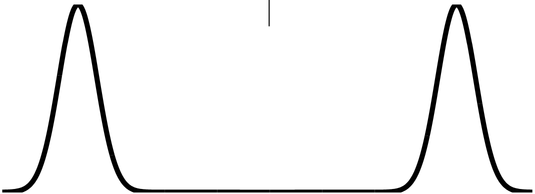
data driven	knowledge driven
adaptive models	



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let the data “speak”

data driven

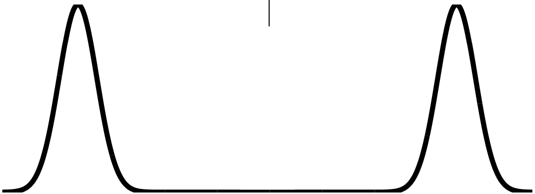
adaptive models

mechanistic modeling

impose physical laws

knowledge driven

differential equations



General Approach

Broadly Speaking: Two approaches to modeling

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let the data "speak"

data driven

adaptive models

digit recognition

mechanistic modeling

impose physical laws

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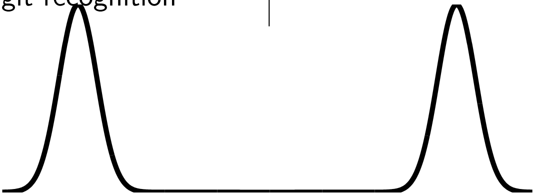
differential equations



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data modeling	*mechanistic modeling*
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data driven	knowledge driven
adaptive models	differential equations
digit recognition	climate, weather models

General Approach

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adaptive models	differential equations
digit recognition	climate, weather models

Weakly Mechanistic

General Approach

Broadly Speaking: Two approaches to modeling

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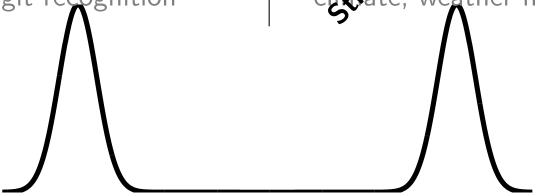
let the data "speak"	impose physical laws
data driven	knowledge driven
adaptive models	differential equations
digit recognition	climate, weather models



Weakly Mechanistic vs Strongly Mechanistic

- Underlying data modeling techniques there are *weakly mechanistic* principles (e.g. smoothness).
- In physics the models are typically *strongly mechanistic*.
- In principle we expect a range of models which vary in the strength of their mechanistic assumptions.
- This work is one part of that spectrum: add further mechanistic ideas to weakly mechanistic models.

Dimensionality Reduction

- Linear relationship between the data, $\mathbf{X} \in \Re^{n \times p}$, and a reduced dimensional representation, $\mathbf{F} \in \Re^{n \times q}$, where $q \ll p$.

$$\mathbf{X} = \mathbf{F}\mathbf{W} + \epsilon,$$

$$\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$$

- Integrate out $\mathbf{F}$, optimize with respect to $\mathbf{W}$.
- For Gaussian prior, $\mathbf{F} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  - and $\Sigma = \sigma^2 \mathbf{I}$ we have probabilistic PCA (**??**).
  - and Σ constrained to be diagonal, we have factor analysis.

Dimensionality Reduction: Temporal Data

- Deal with temporal data with a temporal latent prior.
- Independent Gauss-Markov priors over each $f_i(t)$ leads to : Rauch-Tung-Striebel (RTS) smoother (Kalman filter).
- More generally consider a Gaussian process (GP) prior,

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

Joint Gaussian Process

- Given the covariance functions for $\{f_i(t)\}$ we have an implied covariance function across all $\{x_i(t)\}$—(ML: semi-parametric latent factor model (**?**), Geostatistics: linear model of coregionalization).
- Rauch-Tung-Striebel smoother has been preferred
  - linear computational complexity in n.
  - Advances in sparse approximations have made the general GP framework practical. (**???**).

Mechanical Analogy

Back to Mechanistic Models!

- These models rely on the latent variables to provide the dynamic information.
- We now introduce a further dynamical system with a *mechanistic* inspiration.
- Physical Interpretation:
  - the latent functions, $f_i(t)$ are q forces.
  - We observe the displacement of p springs to the forces.,
  - Interpret system as the force balance equation, $\mathbf{XD} = \mathbf{FS} + \epsilon$.
  - Forces act, e.g. through levers — a matrix of sensitivities, $\mathbf{S} \in \Re^{q \times p}$.
  - Diagonal matrix of spring constants, $\mathbf{D} \in \Re^{p \times p}$.
  - Original System: $\mathbf{W} = \mathbf{SD}^{-1}$.

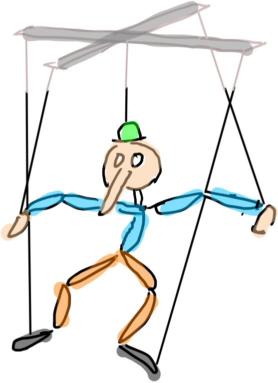
Extend Model

- Add a damper and give the system mass.

$$\mathbf{FS} = \ddot{\mathbf{X}}\mathbf{M} + \dot{\mathbf{X}}\mathbf{C} + \mathbf{XD} + \epsilon.$$

- Now have a second order mechanical system.
- It will exhibit inertia and resonance.
- There are many systems that can also be represented by differential equations.
  - When being forced by latent function(s), $\{f_i(t)\}_{i=1}^q$, we call this a *latent force model*.

Marionette



Mass Spring Damper Analogy

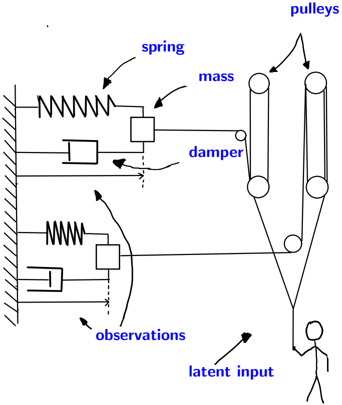
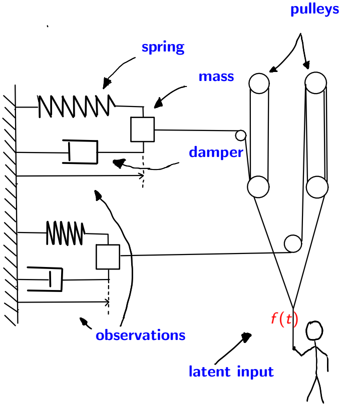


Figure: Mass spring damper analogy, an unobserved force drives multiple oscillators.

Mass Spring Damper Analogy



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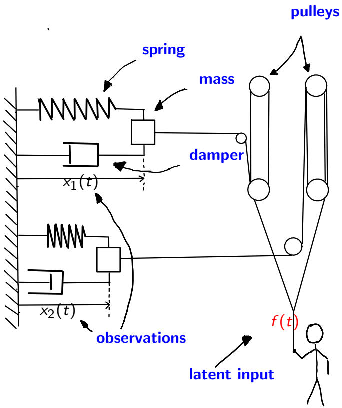

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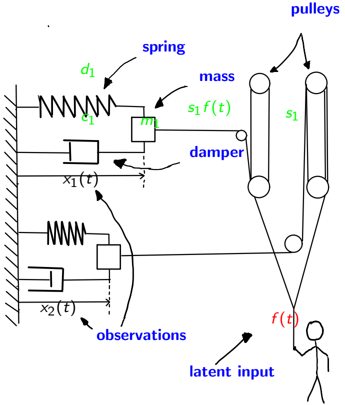

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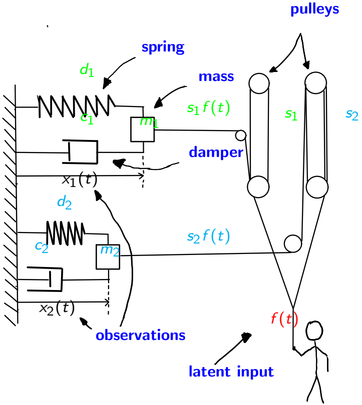

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Gaussian Process priors and Latent Force Models

Driven Harmonic Oscillator

- For Gaussian process we can compute the covariance matrices for the output displacements.
- For one displacement the model is

$$m_k \ddot{x}_k(t) + c_k \dot{x}_k(t) + d_k x_k(t) = b_k + \sum_{i=0}^{q} s_{ik} f_i(t), \qquad (1)$$

  where, m_k is the kth diagonal element from $\mathbf{M}$ and similarly for c_k and d_k. s_{ik} is the i, kth element of $\mathbf{S}$.
- Model the latent forces as q independent, GPs with exponentiated quadratic covariances

$$k_{f_i f_l}(t, t') = \exp\left(-\frac{(t-t')^2}{2\ell_i^2}\right)\delta_{il}.$$

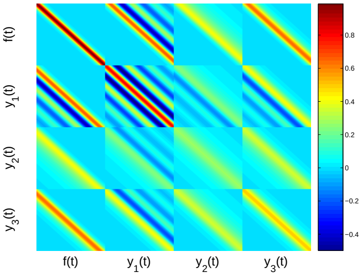
Covariance for ODE Model

- Exponentiated Quadratic Covariance function for $f(t)$

$$x_j(t) = \frac{1}{m_j\omega_j}\sum_{i=1}^{q} s_{ji}\exp(-\alpha_j t)\int_0^t f_i(\tau)\exp(\alpha_j\tau)\sin(\omega_j(t-\tau))\mathrm{d}\tau$$

- Joint distribution for $x_1(t)$, $x_2(t)$, $x_3(t)$ and $f(t)$. Damping ratios:

ζ_1	ζ_2	ζ_3
0.125	2	1



Covariance for ODE Model

- Analogy

$$x = \sum_i \mathbf{e}_i^\top \mathbf{f}_i \quad \mathbf{f}_i \sim \mathcal{N}(\mathbf{0}, \Sigma_i) \rightarrow x \sim \mathcal{N}\left(0, \sum_i \mathbf{e}_i^\top \Sigma_i \mathbf{e}_i\right)$$

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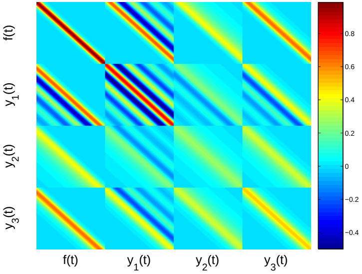

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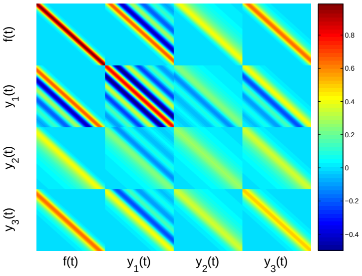

Joint Sampling of $x(t)$ and $f(t)$

- `lfmSample`

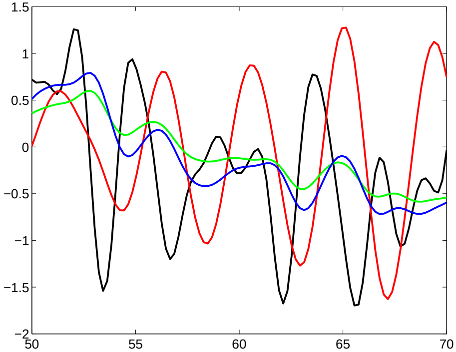

Figure: Joint samples from the ODE covariance, *black*: $f(t)$, *red*: $x_1(t)$ (underdamped), *green*: $x_2(t)$ (overdamped), and *blue*: $x_3(t)$ (critically damped).

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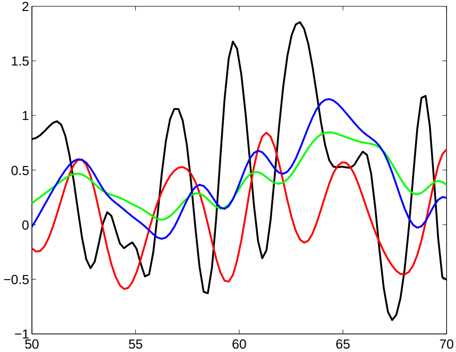

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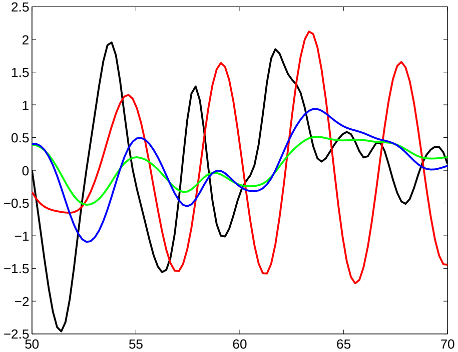

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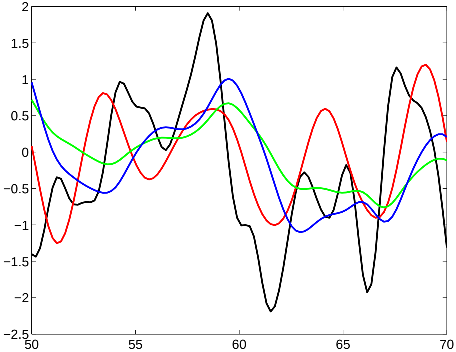

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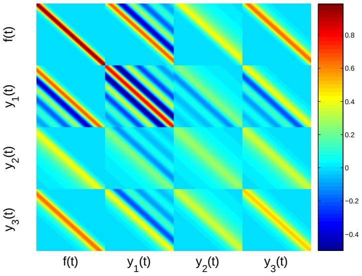

Outline

Example: Motion Capture

Mauricio Alvarez and David Luengo (??)

- Motion capture data: used for animating human motion.
- Multivariate time series of angles representing joint positions.
- Objective: generalize from training data to realistic motions.
- Use 2nd Order Latent Force Model with mass/spring/damper (resistor inductor capacitor) at each joint.

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Prediction of Test Motion

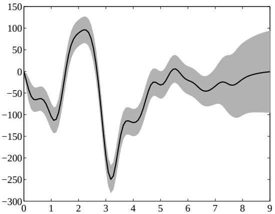
- Model left arm only.
- 3 balancing motions (18, 19, 20) from subject 49.
- 18 and 19 are similar, 20 contains more dramatic movements.
- Train on 18 and 19 and testing on 20
- Data was down-sampled by 32 (from 120 fps).
- Reconstruct motion of left arm for 20 given other movements.
- Compare with GP that predicts left arm angles given other body angles.

Mocap Results

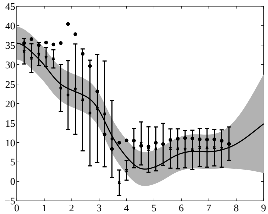
Table: Root mean squared (RMS) angle error for prediction of the left arm's configuration in the motion capture data. Prediction with the latent force model outperforms the prediction with regression for all apart from the radius's angle.

Angle	Latent Force Error	Regression Error
Radius	4.11	4.02
Wrist	6.55	6.65
Hand X rotation	1.82	3.21
Hand Z rotation	2.76	6.14
Thumb X rotation	1.77	3.10
Thumb Z rotation	2.73	6.09

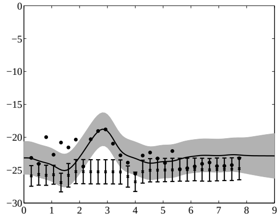
Mocap Results II



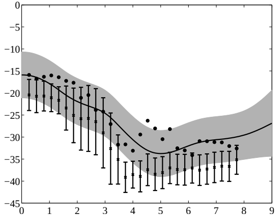
(a) Inferred Latent Force



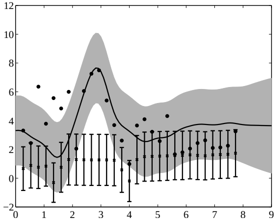
(b) Wrist



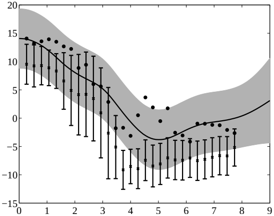
(c) Hand X Rotation



(d) Hand Z Rotation



(e) Thumb X Rotation



(f) Thumb Z Rotation

Figure: Predictions from LFM (solid line, grey error bars) and direct regression

Motion Capture Experiments

- Data set is from the CMU motion capture data base[1].
- Two different types of movements: golf-swing and walking.
- Train on a subset of motions for each movement and test on a different subset.
- This assesses the model's ability to extrapolate.
- For testing: condition on three angles associated to the root nodes and first five and last five frames of the motion.
- Golf-swing use leave one out cross validation on four motions.
- For the walking train on 4 motions and validate on 8 motions.

[1]The CMU Graphics Lab Motion Capture Database was created with funding from NSF EIA-0196217 and is available at `http://mocap.cs.cmu.edu`.

Motion Capture Results

Table: RMSE and R^2 (explained variance) for golf swing and walking

Movement	**Method**	**RMSE**	**R^2 (%)**
Golf swing	IND GP	21.55 ± 2.35	30.99 ± 9.67
	MTGP	21.19 ± 2.18	45.59 ± 7.86
	SLFM	21.52 ± 1.93	49.32 ± 3.03
	LFM	$\mathbf{18.09 \pm 1.30}$	$\mathbf{72.25 \pm 3.08}$
Walking	IND GP	8.03 ± 2.55	30.55 ± 10.64
	MTGP	7.75 ± 2.05	37.77 ± 4.53
	SLFM	7.81 ± 2.00	36.84 ± 4.26
	LFM	$\mathbf{7.23 \pm 2.18}$	$\mathbf{48.15 \pm 5.66}$

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