Neil Lawrence

GPRS 14th February 2014



## Outline

Nonlinear Latent Variable Models

Extensions

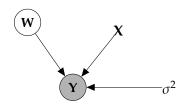
## Outline

Nonlinear Latent Variable Models

Extensions

#### **Dual Probabilistic PCA**

- Define linear-Gaussian relationship between latent variables and data.
- Novel Latent variable approach:
  - ► Define Gaussian prior over *parameteters*, **W**.
  - Integrate out parameters.



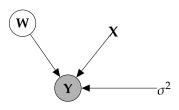
$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:}, \sigma^{2}\mathbf{I})$$

$$p(\mathbf{W}) = \prod_{i=1}^{p} \mathcal{N}\left(\mathbf{w}_{i,:}|\mathbf{0},\mathbf{I}\right)$$

$$p\left(\mathbf{Y}|\mathbf{X}\right) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0},\mathbf{X}\mathbf{X}^{\top} + \sigma^{2}\mathbf{I}\right)$$

#### **Dual Probabilistic PCA**

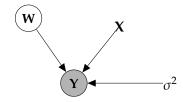
 Inspection of the marginal likelihood shows ...



$$p\left(\mathbf{Y}|\mathbf{X}\right) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0},\mathbf{X}\mathbf{X}^{\top} + \sigma^{2}\mathbf{I}\right)$$

### **Dual Probabilistic PCA**

- Inspection of the marginal likelihood shows ...
  - The covariance matrix is a covariance function.

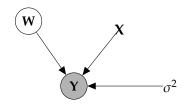


$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K})$$

$$\mathbf{K} = \mathbf{X}\mathbf{X}^{\top} + \sigma^{2}\mathbf{I}$$

#### **Dual Probabilistic PCA**

- Inspection of the marginal likelihood shows ...
  - The covariance matrix is a covariance function.
  - We recognise it as the 'linear kernel'.



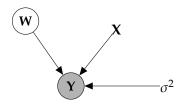
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$$\mathbf{K} = \mathbf{X}\mathbf{X}^{\top} + \sigma^{2}\mathbf{I}$$

This is a product of Gaussian processes with linear kernels.

#### **Dual Probabilistic PCA**

- Inspection of the marginal likelihood shows ...
  - The covariance matrix is a covariance function.
  - We recognise it as the 'linear kernel'.
  - We call this the Gaussian Process Latent Variable model (GP-LVM).



$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K})$$
$$\mathbf{K} = ?$$

Replace linear kernel with non-linear kernel for non-linear model.

## Exponentiated Quadratic (EQ) Covariance

► The EQ covariance has the form  $k_{i,j} = k(\mathbf{x}_{i,:}, \mathbf{x}_{j,:})$ , where

$$k\left(\mathbf{x}_{i,:},\mathbf{x}_{j,:}\right) = \alpha \exp\left(-\frac{\left\|\mathbf{x}_{i,:}-\mathbf{x}_{j,:}\right\|_{2}^{2}}{2\ell^{2}}\right).$$

- ▶ No longer possible to optimise wrt **X** via an eigenvalue problem.
- ▶ Instead find gradients with respect to X,  $\alpha$ ,  $\ell$  and  $\sigma^2$  and optimise using conjugate gradients.

## Outline

Nonlinear Latent Variable Models

Extensions

## Other Topics

- ► Local distance preservation ► Details
- ► Dynamical models ► Details
- ► Hierarchical models ► Details
- ► Bayesian GP-LVM ► Details

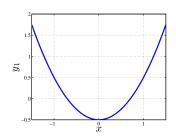
## Local Distance Preservation (Lawrence and Quiñonero Candela, 2006)

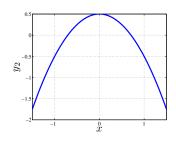
- Most dimensional reduction techniques preserve local distances.
- The GP-LVM does not.
- GP-LVM maps smoothly from latent to data space.
  - ► Points close in latent space are close in data space.
  - This does not imply points close in data space are close in latent space.
- Kernel PCA maps smoothly from data to latent space.
  - ► Points close in data space are close in latent space.
  - This does not imply points close in latent space are close in data space.

## Forward Mapping (demBackMapping in oxford toolbox)

► Mapping from 1-D latent space to 2-D data space.

$$y_1 = x^2 - 0.5$$
,  $y_2 = -x^2 + 0.5$ 

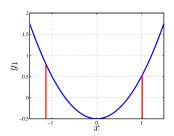


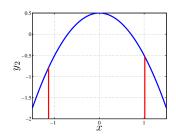


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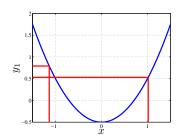


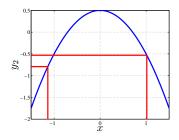


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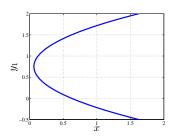


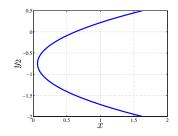


## Backward Mapping (demBackMapping in oxford toolbox)

► Mapping from 2-D data space to 1-D latent.

$$x = 0.5 \left( y_1^2 + y_2^2 + 1 \right)$$

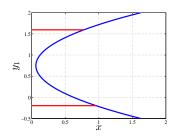


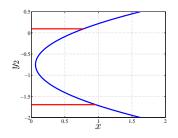


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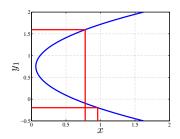


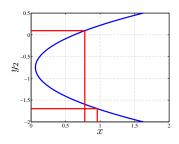


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$$x = 0.5\left(y_1^2 + y_2^2 + 1\right)$$





## NeuroScale

## Multi-Dimensional Scaling with a Mapping

► Lowe and Tipping (1997) made latent positions a function of the data.

$$x_{i,j} = f_j\left(\mathbf{y}_{i,:}; \mathbf{v}\right)$$

- Function was either multi-layer perceptron or a radial basis function network.
- ► Their motivation was different from ours:
  - ► They wanted to add the advantages of a true mapping to multi-dimensional scaling.

## Back Constraints in the GP-LVM

### **Back Constraints**

- We can use the same idea to force the GP-LVM to respect local distances.(Lawrence and Quiñonero Candela, 2006)
  - By constraining each  $x_i$  to be a 'smooth' mapping from  $y_i$  local distances can be respected.
- ► This works because in the GP-LVM we maximise wrt latent variables, we don't integrate out.
- ► Can use any 'smooth' function:
  - 1. Neural network.
  - 2. RBF Network.
  - 3. Kernel based mapping.

# **Optimising BC-GPLVM**

## **Computing Gradients**

► GP-LVM normally proceeds by optimising

$$L\left(\mathbf{X}\right) = \log p\left(\mathbf{Y}|\mathbf{X}\right)$$

with respect to **X** using  $\frac{dL}{d\mathbf{X}}$ .

► The back constraints are of the form

$$x_{i,j} = f_j(\mathbf{y}_{i,:}; \mathbf{v})$$

where  $\mathbf{v}$  are parameters.

► We can compute  $\frac{dI}{dv}$  via chain rule and optimise parameters of mapping.

# Motion Capture Results

demStick1 and demStick3

Figure : The latent space for the motion capture data with (*right*) and without (*left*) back constraints.

# Motion Capture Results

#### demStick1 and demStick3

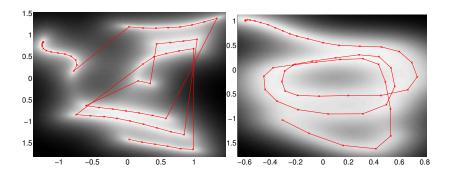
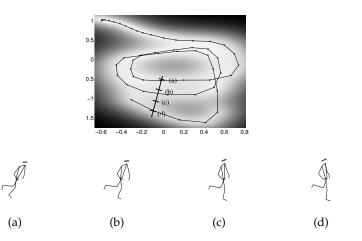


Figure : The latent space for the motion capture data with (*right*) and without (*left*) back constraints.

## Stick Man Results

### demStickResults



Projection into data space from four points in the latent space. The inclination of the runner changes becoming more upright.

# **Adding Dynamics**

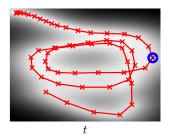
### **MAP Solutions for Dynamics Models**

- Data often has a temporal ordering.
- Markov-based dynamics are often used.
- For the GP-LVM
  - Marginalising such dynamics is intractable.
  - ▶ But: MAP solutions are trivial to implement.
- Many choices: Kalman filter, Markov chains etc..
- ► Wang et al. (2006) suggest using a Gaussian Process.

# Gaussian Process Dynamics

### **GP-LVM** with Dynamics

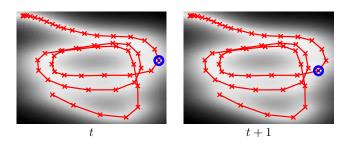
► Autoregressive Gaussian process mapping in latent space between time points.



# Gaussian Process Dynamics

### **GP-LVM** with Dynamics

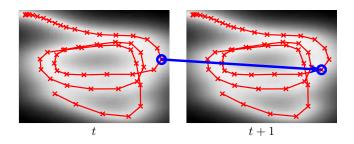
► Autoregressive Gaussian process mapping in latent space between time points.



## Gaussian Process Dynamics

### **GP-LVM** with Dynamics

► Autoregressive Gaussian process mapping in latent space between time points.



# Motion Capture Results

demStick1 and demStick2

Figure: The latent space for the motion capture data without dynamics (*left*), with auto-regressive dynamics (*right*) based on an exponentiated quadratic kernel.

## Motion Capture Results

#### demStick1 and demStick2

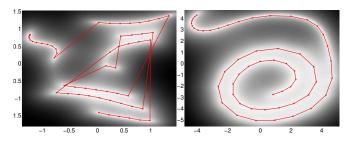
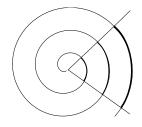


Figure : The latent space for the motion capture data without dynamics (*left*), with auto-regressive dynamics (*right*) based on an exponentiated quadratic kernel.

# Regressive Dynamics

### **Inner Groove Distortion**

- Autoregressive unimodal dynamics,  $p(\mathbf{x}_t|\mathbf{x}_{t-1})$ .
- Forces spiral visualisation.
- Poorer model due to inner groove distortion.



# Regressive Dynamics

#### **Direct use of Time Variable**

- ► Instead of auto-regressive dynamics, consider regressive dynamics.
- ► Take **t** as an input, use a prior  $p(\mathbf{X}|\mathbf{t})$ .
- ▶ User a Gaussian process prior for p(X|t).
- ► Also allows us to consider variable sample rate data.

# Motion Capture Results

demStick1, demStick2 and demStick5

Figure: The latent space for the motion capture data without dynamics (*left*), with auto-regressive dynamics (*middle*) and with regressive dynamics (*right*) based on an exponentiated quadratic kernel.

## Motion Capture Results

### demStick1, demStick2 and demStick5

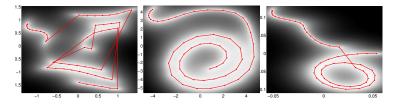


Figure: The latent space for the motion capture data without dynamics (*left*), with auto-regressive dynamics (*middle*) and with regressive dynamics (*right*) based on an exponentiated quadratic kernel.



## Hierarchical GP-LVM

(Lawrence and Moore, 2007)

### **Stacking Gaussian Processes**

- ► Regressive dynamics provides a simple hierarchy.
  - ▶ The input space of the GP is governed by another GP.
- By stacking GPs we can consider more complex hierarchies.
- Ideally we should marginalise latent spaces
  - ► In practice we seek MAP solutions.

# Two Correlated Subjects

(Lawrence and Moore, 2007)

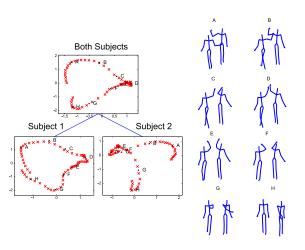


Figure: Hierarchical model of a 'high five'.

# Within Subject Hierarchy

(Lawrence and Moore, 2007)

### **Decomposition of Body**

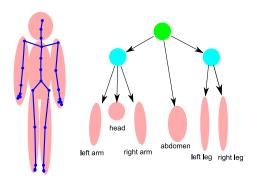


Figure: Decomposition of a subject.

### Single Subject Run/Walk

(Lawrence and Moore, 2007)

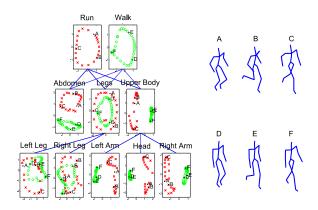


Figure: Hierarchical model of a walk and a run.

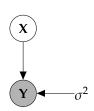


# Selecting Data Dimensionality

- ► GP-LVM Provides probabilistic non-linear dimensionality reduction.
- ▶ How to select the dimensionality?
- ▶ Need to estimate marginal likelihood.
- ► In standard GP-LVM it increases with increasing *q*.

#### **Bayesian GP-LVM**

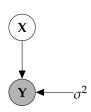
Start with a standard GP-LVM.



$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K})$$

#### **Bayesian GP-LVM**

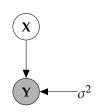
- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - ► Define Gaussian prior over *latent space*, **X**.



$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K})$$

#### **Bayesian GP-LVM**

- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - Define Gaussian prior over latent space, X.
  - ► Integrate out *latent* variables.

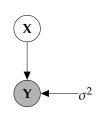


$$p\left(\mathbf{Y}|\mathbf{X}\right) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0},\mathbf{K}\right)$$

$$p\left(\mathbf{X}\right) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0},\alpha_{i}^{-2}\mathbf{I}\right)$$

#### **Bayesian GP-LVM**

- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - Define Gaussian prior over latent space, X.
  - ► Integrate out *latent* variables.
  - Unfortunately integration is intractable.



$$p\left(\mathbf{Y}|\mathbf{X}\right) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0},\mathbf{K}\right)$$

$$p(\mathbf{X}) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0}, \alpha_{i}^{-2}\mathbf{I}\right)$$
$$p(\mathbf{Y}|\boldsymbol{\alpha}) =??$$

### Standard Variational Approach Fails

▶ Standard variational bound has the form:

$$\mathcal{L} = \left\langle \log p(\mathbf{y}|\mathbf{X}) \right\rangle_{q(\mathbf{X})} + \mathrm{KL}\left(q(\mathbf{X}) \parallel p(\mathbf{X})\right)$$

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► Requires expectation of  $\log p(y|X)$  under q(X).

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

# Standard Variational Approach Fails

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Extremely difficult to compute because K<sub>f,f</sub> is dependent on X and appears in the inverse.

Consider collapsed variational bound,

$$p(\mathbf{y}) \ge \prod_{i=1}^{n} c_i \int \mathcal{N}(\mathbf{y}|\langle \mathbf{f} \rangle, \sigma^2 \mathbf{I}) p(\mathbf{u}) d\mathbf{u}$$

Consider collapsed variational bound,

$$p(\mathbf{y}|\mathbf{X}) \ge \prod_{i=1}^{n} c_i \int \mathcal{N}(\mathbf{y}|\langle \mathbf{f} \rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^2 \mathbf{I}) p(\mathbf{u}) d\mathbf{u}$$

► Consider collapsed variational bound,

$$\int p(\mathbf{y}|\mathbf{X})p(\mathbf{X})d\mathbf{X} \geq \int \prod_{i=1}^{n} c_{i} \mathcal{N}\left(\mathbf{y}|\langle \mathbf{f} \rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^{2} \mathbf{I}\right) p(\mathbf{X})d\mathbf{X}p(\mathbf{u})d\mathbf{u}$$

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► Apply variational lower bound to the inner integral.

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► Apply variational lower bound to the inner integral.

$$\int \prod_{i=1}^{n} c_{i} \mathcal{N}\left(\mathbf{y} | \langle \mathbf{f} \rangle_{p(\mathbf{f} | \mathbf{u}, \mathbf{X})}, \sigma^{2} \mathbf{I}\right) p(\mathbf{X}) d\mathbf{X}$$

$$\geq \left\langle \sum_{i=1}^{n} \log c_{i} \right\rangle_{q(\mathbf{X})} + \left\langle \log \mathcal{N}\left(\mathbf{y} | \langle \mathbf{f} \rangle_{p(\mathbf{f} | \mathbf{u}, \mathbf{X})}, \sigma^{2} \mathbf{I}\right) \right\rangle_{q(\mathbf{X})} + KL\left(q(\mathbf{X}) \parallel p(\mathbf{X})\right)$$

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$$\geq \left\langle \sum_{i=1}^{n} \log c_{i} \right\rangle_{q(\mathbf{X})}$$

$$+ \left\langle \log \mathcal{N}\left(\mathbf{y} | \langle \mathbf{f} \rangle_{p(\mathbf{f} | \mathbf{u}, \mathbf{X})}, \sigma^{2} \mathbf{I}\right) \right\rangle_{q(\mathbf{X})}$$

$$+ KL\left(q(\mathbf{X}) || p(\mathbf{X})\right)$$

• Which is analytically tractable for Gaussian  $q(\mathbf{X})$  and some covariance functions.

# **Required Expectations**

▶ Need expectations under q(X) of:

$$\log c_i = \frac{1}{2\sigma^2} \left[ k_{i,i} - \mathbf{k}_{i,\mathbf{u}}^{\mathsf{T}} \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{k}_{i,\mathbf{u}} \right]$$

and

$$\log \mathcal{N}\left(\mathbf{y}|\langle \mathbf{f}\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{Y})}, \sigma^{2}\mathbf{I}\right) = -\frac{1}{2}\log 2\pi\sigma^{2} - \frac{1}{2\sigma^{2}}\left(y_{i} - \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\right)^{2}$$

► This requires the expectations

$$\left\langle \mathbf{K}_{\mathbf{f},\mathbf{u}}\right\rangle _{q(\mathbf{X})}$$

and

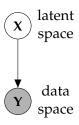
$$\left\langle \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{u},\mathbf{f}}\right\rangle _{q(\mathbf{X})}$$

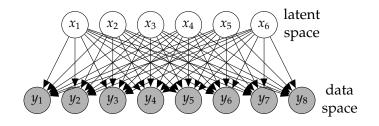
which can be computed analytically for some covariance functions.

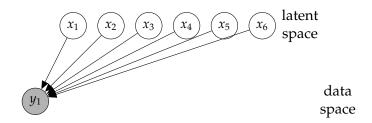
# **Priors for Latent Space**

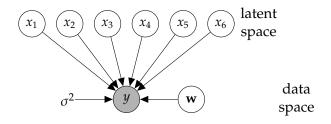
#### Titsias and Lawrence (2010)

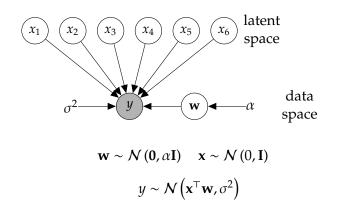
- ▶ Variational marginalization of X allows us to learn parameters of p(X).
- Standard GP-LVM where X learnt by MAP, this is not possible (see e.g. Wang et al., 2008).
- ► First example: learn the dimensionality of latent space.

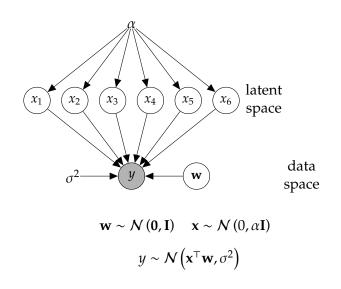


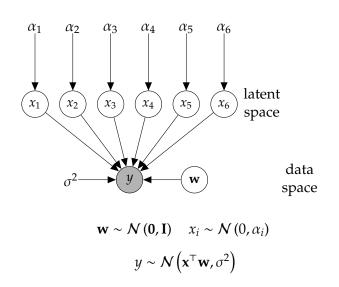


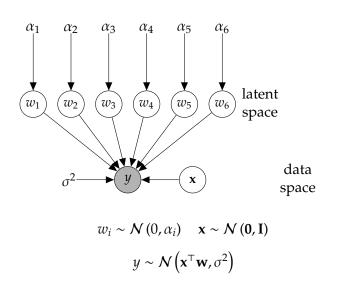












# Non-linear $f(\mathbf{x})$

► In linear case equivalence because  $f(\mathbf{x}) = \mathbf{w}^{\top}\mathbf{x}$ 

$$p(w_i) \sim \mathcal{N}(\mathbf{0}, \alpha_i)$$

- ► In non linear case, need to scale columns of X in prior for f(x).
- ► This implies scaling columns of **X** in covariance function

$$k(\mathbf{x}_{i,:},\mathbf{x}_{j,:}) = \exp\left(-\frac{1}{2}(\mathbf{x}_{:,i} - \mathbf{x}_{:,j})^{\top}\mathbf{A}(\mathbf{x}_{:,i} - \mathbf{x}_{:,j})\right)$$

**A** is diagonal with elements  $\alpha_i^2$ . Now keep prior spherical

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

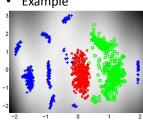
► Covariance functions of this type are known as ARD (see e.g. Neal, 1996; MacKay, 2003; Rasmussen and Williams, 2006).

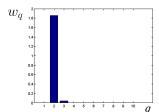
### Automatic dimensionality detection

Achieved by employing an Automatic Relevance Determination (ARD) covariance function for the prior on the GP mapping

• 
$$f\sim GP(\mathbf{0},k_f)$$
 with 
$$k_f\left(\mathbf{x}_i,\mathbf{x}_j\right)=\sigma^2\exp\left(-\frac{1}{2}\sum_{q=1}^Qw_q\left(x_{i,q}-x_{j,q}\right)^2\right)$$

Example





### **Applications**

#### **Style Based Inverse Kinematics**

► Facilitating animation through modeling human motion (Grochow et al., 2004)

#### Tracking

► Tracking using human motion models (Urtasun et al., 2005, 2006)

#### **Assisted Animation**

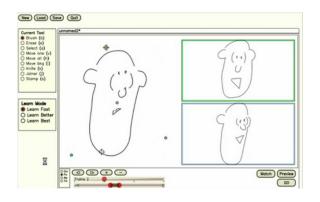
► Generalizing drawings for animation (Baxter and Anjyo, 2006)

#### **Shape Models**

► Inferring shape (e.g. pose from silhouette). (Ek et al., 2008b,a; Priacuriu and Reid, 2011a,b)

### Example: Latent Doodle Space

(Baxter and Anjyo, 2006)



http://vimeo.com/3235882

# Example: Latent Doodle Space

(Baxter and Anjyo, 2006)

#### Generalization with much less Data than Dimensions

- Powerful uncertainly handling of GPs leads to surprising properties.
- ▶ Non-linear models can be used where there are fewer data points than dimensions *without overfitting*.

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