Unsupervised Learning with Gaussian Processes

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GPSS
14th September 2015

Outline

Motivating Example

Linear Dimensionality Reduction

Non-linear Dimensionality Reduction

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Motivation for Non-Linear Dimensionality Reduction

USPS Data Set Handwritten Digit

- 3648 Dimensions
  - 64 rows by 57 columns

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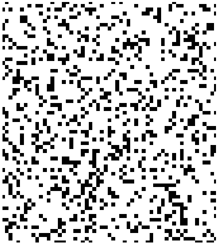

Motivation for Non-Linear Dimensionality Reduction

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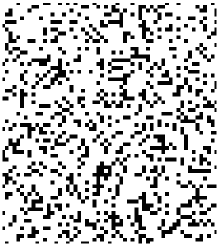

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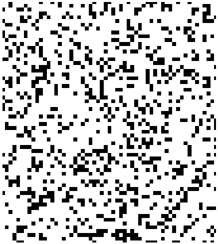

Simple Model of Digit

Rotate a 'Prototype'

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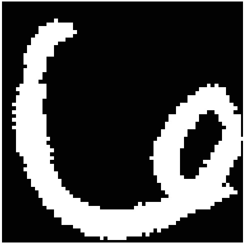

MATLAB Demo

```
demDigitsManifold([1 2], 'all')
```

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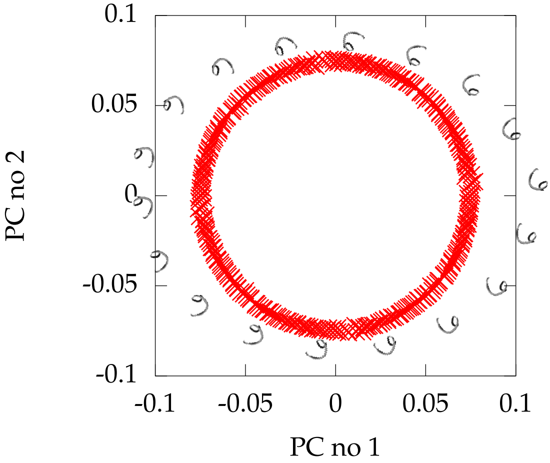

MATLAB Demo

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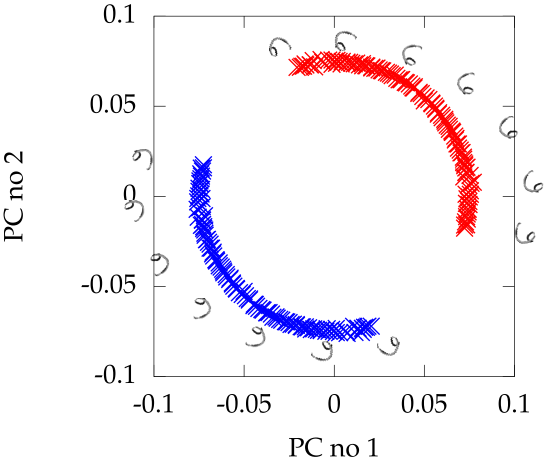
demDigitsManifold([1 2], 'sixnine')
```



Low Dimensional Manifolds

Pure Rotation is too Simple

- In practice the data may undergo several distortions.
  - *e.g.* digits undergo 'thinning', translation and rotation.
- For data with 'structure':
  - we expect fewer distortions than dimensions;
  - we therefore expect the data to live on a lower dimensional manifold.
- Conclusion: deal with high dimensional data by looking for lower dimensional non-linear embedding.

Outline

Notation

q— dimension of latent/embedded space
p— dimension of data space
n— number of data points

$$\text{data, } \mathbf{Y} = [\mathbf{y}_{1,:}, \ldots, \mathbf{y}_{n,:}]^\top = \left[\mathbf{y}_{:,1}, \ldots, \mathbf{y}_{:,p}\right] \in \Re^{n\times p}$$
$$\textit{centred} \text{ data, } \hat{\mathbf{Y}} = [\hat{\mathbf{y}}_{1,:}, \ldots, \hat{\mathbf{y}}_{n,:}]^\top = \left[\hat{\mathbf{y}}_{:,1}, \ldots, \hat{\mathbf{y}}_{:,p}\right] \in \Re^{n\times p},$$
$$\hat{\mathbf{y}}_{i,:} = \mathbf{y}_{i,:} - \boldsymbol{\mu}$$
$$\text{latent variables, } \mathbf{X} = [\mathbf{x}_{1,:}, \ldots, \mathbf{x}_{n,:}]^\top = \left[\mathbf{x}_{:,1}, \ldots, \mathbf{x}_{:,q}\right] \in \Re^{n\times q}$$
$$\text{mapping matrix, } \mathbf{W} \in \Re^{p\times q}$$

$\mathbf{a}_{i,:}$ is a vector from the ith row of a given matrix $\mathbf{A}$
$\mathbf{a}_{:,j}$ is a vector from the jth row of a given matrix $\mathbf{A}$

Reading Notation

$\mathbf{X}$ and $\mathbf{Y}$ are *design matrices*

- Data covariance given by $\frac{1}{n}\hat{\mathbf{Y}}^\top\hat{\mathbf{Y}}$

$$\text{cov}\left(\mathbf{Y}\right) = \frac{1}{n}\sum_{i=1}^{n}\hat{\mathbf{y}}_{i,:}\hat{\mathbf{y}}_{i,:}^\top = \frac{1}{n}\hat{\mathbf{Y}}^\top\hat{\mathbf{Y}} = \mathbf{S}.$$

- Inner product matrix given by $\mathbf{Y}\mathbf{Y}^\top$

$$\mathbf{K} = \left(k_{i,j}\right)_{i,j}, \qquad k_{i,j} = \mathbf{y}_{i,:}^\top\mathbf{y}_{j,:}$$

Linear Dimensionality Reduction

- Find a lower dimensional plane embedded in a higher dimensional space.
- The plane is described by the matrix $\mathbf{W} \in \Re^{p\times q}$.

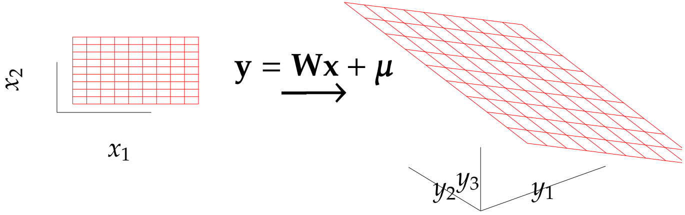


Figure: Mapping a two dimensional plane to a higher dimensional space in a linear way. Data are generated by corrupting points on the plane with noise.

Linear Latent Variable Model

- Represent data, $\mathbf{Y}$, with a lower dimensional set of latent variables $\mathbf{X}$.
- Assume a linear relationship of the form

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

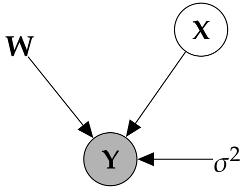
where

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

Linear Latent Variable Model

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.



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

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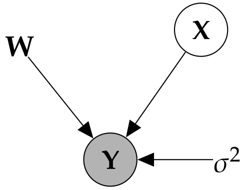

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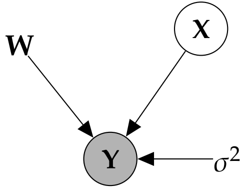

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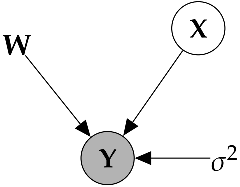

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$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:} + \boldsymbol{\epsilon}_{i,:}, \quad \mathbf{x}_{i,:} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right)$$

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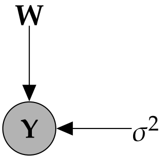

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where $\mathbf{R}$ is an arbitrary rotation matrix.

Outline

Difficulty for Probabilistic Approaches

- Propagate a probability distribution through a non-linear mapping.
- Normalisation of distribution becomes intractable.

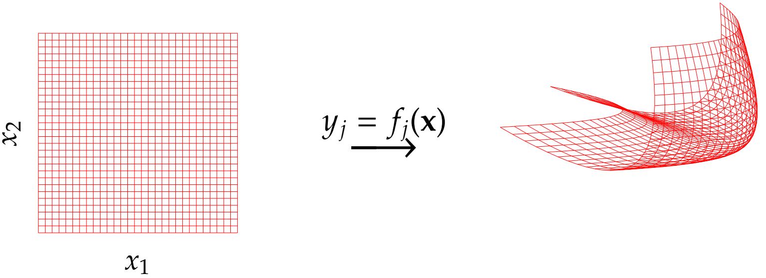


Figure: A three dimensional manifold formed by mapping from a two dimensional space to a three dimensional space.

Difficulty for Probabilistic Approaches

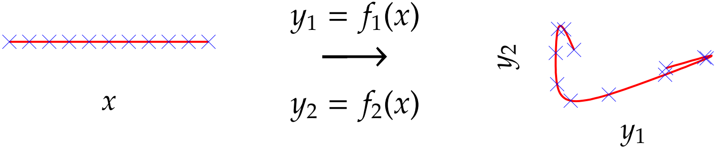


Figure: A string in two dimensions, formed by mapping from one dimension, x, line to a two dimensional space, $[y_1, \ y_2]$ using nonlinear functions $f_1(\cdot)$ and $f_2(\cdot)$.

Difficulty for Probabilistic Approaches

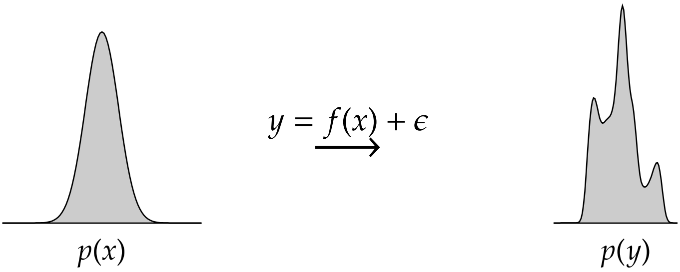
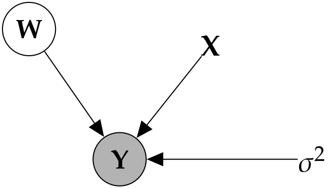


Figure: A Gaussian distribution propagated through a non-linear mapping. $y_i = f(x_i) + \epsilon_i$. $\epsilon \sim \mathcal{N}\left(0, 0.2^2\right)$ and $f(\cdot)$ uses RBF basis, 100 centres between -4 and 4 and $\ell = 0.1$. New distribution over y (right) is multimodal and difficult to normalize.

Linear Latent Variable Model III

Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.



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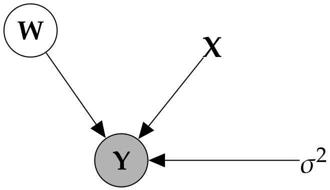

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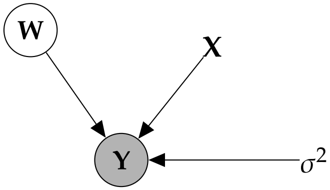

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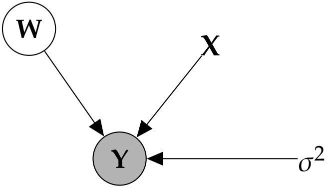

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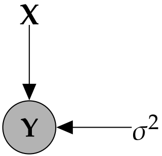

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$$\log p\left(\mathbf{Y}|\mathbf{W}\right) = -\frac{n}{2}\log\left|\mathbf{C}\right| - \frac{1}{2}\mathrm{tr}\left(\mathbf{C}^{-1}\mathbf{Y}^{\top}\mathbf{Y}\right) + \text{const.}$$

If $\mathbf{U}_q$ are first q principal eigenvectors of $n^{-1}\mathbf{Y}^{\top}\mathbf{Y}$ and the corresponding eigenvalues are $\boldsymbol{\Lambda}_q$,

$$\mathbf{W} = \mathbf{U}_q\mathbf{L}\mathbf{R}^{\top}, \quad \mathbf{L} = \left(\boldsymbol{\Lambda}_q - \sigma^2\mathbf{I}\right)^{\frac{1}{2}}$$

where $\mathbf{R}$ is an arbitrary rotation matrix.

Equivalence of Formulations

The Eigenvalue Problems are equivalent

- Solution for Probabilistic PCA (solves for the mapping)

$$\mathbf{Y}^\top \mathbf{Y} \mathbf{U}_q = \mathbf{U}_q \mathbf{\Lambda}_q \qquad \mathbf{W} = \mathbf{U}_q \mathbf{L} \mathbf{R}^\top$$

- Solution for Dual Probabilistic PCA (solves for the latent positions)

$$\mathbf{Y} \mathbf{Y}^\top \mathbf{U}'_q = \mathbf{U}'_q \mathbf{\Lambda}_q \qquad \mathbf{X} = \mathbf{U}'_q \mathbf{L} \mathbf{R}^\top$$

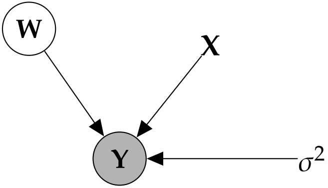
- Equivalence is from

$$\mathbf{U}_q = \mathbf{Y}^\top \mathbf{U}'_q \mathbf{\Lambda}_q^{-\frac{1}{2}}$$

Non-Linear Latent Variable Model

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*.



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

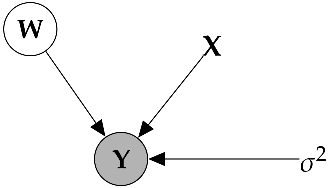
$$p(\mathbf{W}) = \prod_{i=1}^{p} \mathcal{N}\left(\mathbf{w}_{i,:}|\mathbf{0},\mathbf{I}\right)$$

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

Non-Linear Latent Variable Model

Dual Probabilistic PCA

- Inspection of the marginal likelihood shows ...

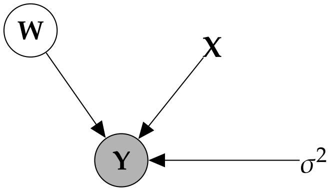


$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{X}\mathbf{X}^{\top} + \sigma^2\mathbf{I}\right)$$

Non-Linear Latent Variable Model

Dual Probabilistic PCA

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



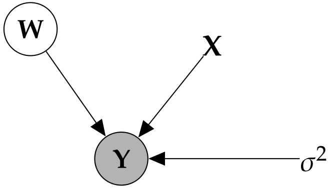
$$p\left(\mathbf{Y}|\mathbf{X}\right) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

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

Non-Linear Latent Variable Model

Dual Probabilistic PCA

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



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

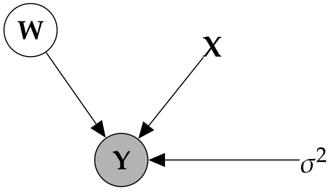
$$\mathbf{K} = \mathbf{X}\mathbf{X}^{\top} + \sigma^2\mathbf{I}$$

This is a product of Gaussian processes with linear kernels.

Non-Linear Latent Variable Model

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).



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

$$\mathbf{K} = ?$$

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

Exponentiated Quadratic (EQ) Covariance

- The EQ covariance has the form $k_{i,j} = k\left(\mathbf{x}_{i,:}, \mathbf{x}_{j,:}\right)$, 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 $\mathbf{X}$ via an eigenvalue problem.
- Instead find gradients with respect to $\mathbf{X}, \alpha, \ell$ and σ^2 and optimise using conjugate gradients.

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)

Stick Man

Generalization with 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*.
- Example: Modelling a stick man in 102 dimensions with 55 data points!

`demStick1`

Figure: The latent space for the stick man motion capture data.

Stick Man II

`demStick1`

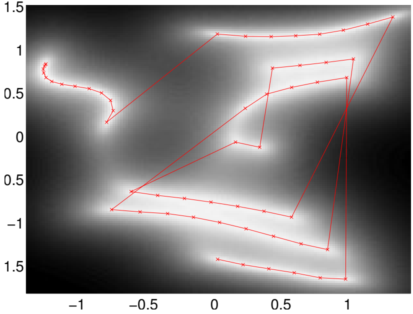
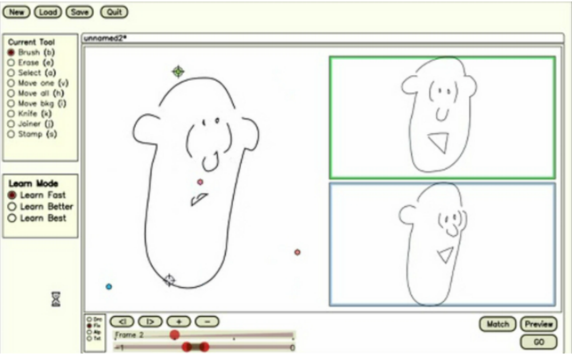


Figure: The latent space for the stick man motion capture data.

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*.

References I

W. V. Baxter and K.-I. Anjyo. Latent doodle space. In *EUROGRAPHICS*, volume 25, pages 477–485, Vienna, Austria, September 4-8 2006.

C. H. Ek, J. Rihan, P. Torr, G. Rogez, and N. D. Lawrence. Ambiguity modeling in latent spaces. In A. Popescu-Belis and R. Stiefelhagen, editors, *Machine Learning for Multimodal Interaction (MLMI 2008)*, LNCS, pages 62–73. Springer-Verlag, 28–30 June 2008a. [PDF].

C. H. Ek, P. H. Torr, and N. D. Lawrence. Gaussian process latent variable models for human pose estimation. In A. Popescu-Belis, S. Renals, and H. Bourlard, editors, *Machine Learning for Multimodal Interaction (MLMI 2007)*, volume 4892 of *LNCS*, pages 132–143, Brno, Czech Republic, 2008b. Springer-Verlag. [PDF].

K. Grochow, S. L. Martin, A. Hertzmann, and Z. Popovic. Style-based inverse kinematics. In *ACM Transactions on Graphics (SIGGRAPH 2004)*, pages 522–531, 2004.

N. D. Lawrence. Gaussian process models for visualisation of high dimensional data. In S. Thrun, L. Saul, and B. Schölkopf, editors, *Advances in Neural Information Processing Systems*, volume 16, pages 329–336, Cambridge, MA, 2004. MIT Press.

N. D. Lawrence. Probabilistic non-linear principal component analysis with Gaussian process latent variable models. *Journal of Machine Learning Research*, 6:1783–1816, 11 2005.

V. Priacuriu and I. D. Reid. Nonlinear shape manifolds as shape priors in level set segmentation and tracking. In *Proceedings of the IEEE Computer Society Conference on Computer Vision and Pattern Recognition*, 2011a.

V. Priacuriu and I. D. Reid. Shared shape spaces. In *IEEE International Conference on Computer Vision (ICCV)*, 2011b.

M. E. Tipping and C. M. Bishop. Probabilistic principal component analysis. *Journal of the Royal Statistical Society, B*, 6 (3):611–622, 1999. [PDF]. [DOI].

R. Urtasun, D. J. Fleet, and P. Fua. 3D people tracking with Gaussian process dynamical models. In *Proceedings of the IEEE Computer Society Conference on Computer Vision and Pattern Recognition*, pages 238–245, New York, U.S.A., 17–22 Jun. 2006. IEEE Computer Society Press.

R. Urtasun, D. J. Fleet, A. Hertzmann, and P. Fua. Priors for people tracking from small training sets. In *IEEE International Conference on Computer Vision (ICCV)*, pages 403–410, Bejing, China, 17–21 Oct. 2005. IEEE Computer Society Press.