GTM: The Generative Topographic Mapping

Presenter
Folami Alamudun

Authors
Christopher M. Bishop
Markus Svensen
Christopher K.I. Williams
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Chris Bishop is Chief Research Scientist at Microsoft Research Cambridge, and Professor of Computer Science at the University of Edinburgh.

He is a Fellow of the Royal Academy of Engineering, a Fellow of the Royal Society of Edinburgh, and a Fellow of Darwin College Cambridge. His research interests include machine learning and its applications.

Related work
What?
- Generative Topographic mapping (GTM) is a novel non-linear latent variable model.

Why?
- GTM seeks an explanation to the behavior of a number of data variables in terms of a smaller number of latent variables.

How?
- GTM allows for a non-linear relationship between latent and observed variables.

Introduction
What is a latent variable model?
- Methodic representation of multidimensional data in fewer dimensions using latent variables

What are other examples of latent variable models?
- Factor Analysis
- Probabilistic Principal Component Analysis.
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• The goal of GTM is to define a probability distribution, \( p(t) \), over D-dimensional space (D-space) \( t = (t_1, t_2, t_3, \ldots, t_D) \) in terms of latent variables \( x = (x_1, x_2, x_3, \ldots, x_L) \).

• GTM uses a non-linear, parametric function \( y(x, W) \) which maps every point in the latent space to a point in the data space
  - from L-dimensional L-space (\( x \in \mathbb{R}^L \))
  - to a corresponding point (\( y \in \mathbb{R}^D \)) in D-space

where:
  - \( L < D \)

**GTM Model**
GTM Model
We define probability distribution over L-space as \( p(x) \), then probability distribution over D-space convolved with an isotropic Gaussian noise distribution can be given by:

\[
p(t \mid x, W, \beta) = \mathcal{N}(y(x, W), \beta) \frac{1}{2} \exp \left\{ -\frac{\beta}{2} \| y(x, W) - t \|^2 \right\}
\]

where
- \( T \) is a point in data space; and
- \( \beta^{-1} \) denotes the noise variance.
For a given value of $W$, the distribution in D-space is given by:

$$p(t | W, \beta) = \int p(t | x, W, \beta) p(x) dx$$

For a given dataset of N data points, $D = (t_1, t_2, t_3, ..., t_D)$, the parameter matrix $W$, and inverse matrix $\beta$ are obtained by maximizing the log likelihood $\mathcal{L}(W, \beta)$ given by:

$$\mathcal{L}(W, \beta) = \ln \prod_{n=1}^{N} p(t_n | W, \beta)$$

GTM Model
For analytical tractability, we use a set of $K$ equally weighted delta functions on a regular grid to represent $p(x)$. The log likelihood function becomes:

$$
\mathcal{L}(\mathbf{w}, \beta) = \sum_{n=1}^{N} \ln \left\{ \frac{1}{K} \sum_{k} p(t_n | x_k, \mathbf{w}, \beta) \right\}
$$

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The Expectation maximization algorithm works in two steps:

- **E-step**: Uses $W_{\text{old}}$ and $\beta_{\text{old}}$ to calculate the responsibility (posterior probabilities) for each Gaussian component $i$ for all data points $t_n$.

\[
E_{\text{comp}}(W, \beta) = \sum_{n=1}^{N} \sum_{i=1}^{K} R_{j,n} \ln(W_{\text{old}i}, \beta_{\text{old}i}) \ln(p(t_n|x_i, W, \beta))
\]
\[ y_d(x, W) = \sum_{m}^{M} \phi_m(x) w_{md} \]

- \( W \) is a \( M \times D \) matrix containing weight and bias parameters.

\[
\phi_m(x) = \begin{cases} 
\exp \left\{ -\frac{\|x - \mu_m\|^2}{2\sigma^2} \right\} & \text{if } m \leq M_{NL}, \\
x^l & \text{if } m = M_{NL} + l, \ l = 1, \ldots, L \\
1 & \text{if } m = M_{NL} + L + 1 = M, 
\end{cases}
\]

- \( M_{NL} \) non-linear basis functions in the form of non-normalized Gaussian basis functions.
- \( L \) linear basis functions - for capturing linear trends in the data.
- One fixed basis function that allows the corresponding weights to act as biases.

**EM Algorithm for GTM**
• M-step calculates $W_{\text{new}}$ and $\beta_{\text{new}}$ from the maximized log likelihood $\mathcal{L}(W,\beta)$ equations given by:
  
  $\phi^T G_{\text{old}} \phi W_{\text{new}}^T = \phi^T R_{\text{old}} T$

  $\beta_{\text{new}}$ from

  \[
  \frac{1}{\beta_{\text{new}}} = \frac{1}{ND} \sum_{n=1}^{N} \sum_{k=1}^{K} R_{kn} (W_{\text{old}}, \beta_{\text{old}}) ||W_{\text{new}} \phi(x_i) - t_n||^2
  \]

  $T$ is an N x D matrix with elements $T_{nk}$;

  $R$ is a K x N matrix with elements $R_{in}$;

  $G$ is a K x K diagonal matrix:

  $G_{tt} = \sum_{n=1}^{N} R_{tn}(W, \beta)$

**EM Algorithm for GTM**
• Generate the grid of latent points \( \{x_k\} \ k = 1,\ldots,K \)
• Generate the grid of basis function centres \( \{\mu_m\} \ m = 1,\ldots, M \)
• Select the basis function width \( \sigma \)
• Compute the matrix of basis function activations \( \Phi \)
• Initialize \( W \) randomly or using PCA
• Initialize \( \beta \)
• Train by alternating between E-step and M-step.
  ◦ Evaluate log likelihood at the end of each cycle for convergence.

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• A potential application for GTM is visualization

• By calculating $W^*$ and $\beta^*$, GTM defines the probability distribution in the data space conditioned on the latent variable, $p(t|x_k)$, $k = 1,...,K$.

• Bayes Theorem can be used to calculate the corresponding posterior distribution in latent space for any point in data space, $p(x_k|t)$.
• We can plot \( p(x_k|t) \) against \( x_k \);

• Alternatively, for each data point \( t_n \), we can plot the entire data set by calculating:
  
  ◦ the posterior mode projection of the distribution:
    
    \[
    x_{n_{\text{mode}}} = \arg\max_{x_k} p(x_k|t_n)
    \]
    
    OR
  
  ◦ the posterior mean projection of the distribution:
    
    \[
    x_{n_{\text{mean}}} = \sum_{k} x_k p(x_k|t_n)
    \]
The following illustrates the GTM learning process:
- GTM 1-D latent variable learns to model a 2-D curved line.
- The plots show the density model in data space.

Experimental Results
Density model in data space after 2\textsuperscript{nd} and 4\textsuperscript{th} iteration.

Experimental Results
Density model in data space after 8\textsuperscript{th} and 15\textsuperscript{th} iteration

Experimental Results
The following illustrates GTM on 3-phase pipe flow data. GTM uses synthetically generated data simulating flow in a pipeline transporting a mixture of gas, oil and water.

A cross sectional view of three different configurations
Left to right: Homogeneous, Annular and Stratified

Experimental Results
Left: posterior-mean projection of the data in latent space of the PCA initialized GTM before training.
Right: Corresponding plot after training.

Experimental Results
<table>
<thead>
<tr>
<th>SOM</th>
<th>GTM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Doesn’t optimize an objective function. Such a function doesn’t exist</td>
<td>It optimizes an objective function (log-likelihood function).</td>
</tr>
<tr>
<td>There is no general guarantee that the algorithm will converge</td>
<td>The EM-algorithm is guaranteed to converge to a maxima of the likelihood function.</td>
</tr>
<tr>
<td>There is no theoretical framework based on which appropriate values for the model parameters can be chosen</td>
<td>Uses Bayesian statistical theory to derive methods for treating model parameters.</td>
</tr>
<tr>
<td>There is no logical means for comparing one SOM model to another or to different architectures.</td>
<td>The likelihood is a measure that can serve as a bases for comparing GTM model to other generative models.</td>
</tr>
<tr>
<td>The mapping from topographic space to data space in the original SOM is only defined at locations of the nodes.</td>
<td>GTM defines a continuous manifold in the data space.</td>
</tr>
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Relationship to other Models
• **Elastic Net Algorithm:**
  ◦ A Gaussian mixture that encourages centers to follow a locally 1-D, globally cyclic structure.
  ◦ Does not define a continuous data space manifold

• **Principal Curves:**
  ◦ Similar to SOM. Projects each data point to a single point on the curve.
  ◦ Uses Gaussian mixture equal to number of data points and a well defined likelihood function trained by the EM algorithm.
Benefits to the probabilistic model used in GTM:

- Handling missing data values by simple modification of the EM algorithm
- GTM can be used for visualization of data from the modeled distribution
- GTM models can be combined:
  - \( P(t) = \Sigma_r P(r)p(t|r) \)
    - \( P(t|r) \) represents the \( r^{th} \) model.
- GTM can be generalized, extended and adapted within the framework of probability theory

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