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Latent Gaussian Processes for Distribution Estimation of Multivariate Categorical Data

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Distribution Estimation

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- Distribution estimation of categorical data $\{y_n \mid n = 1, ..., N\}$ with $y_n \in \{1, ..., K\}$ is easy.
- But learning a distribution

$$P(\mathbf{y})$$

from vectors of categorical data,

$$\{\mathbf{y}_n = (y_{n1}, ..., y_{nD}) \mid n = 1, ..., N\}$$

with

$$y_{nd} \in \{1, ..., K\},$$

is much more difficult.

Multivariate Categorical Data

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Multivariate Categorical Data

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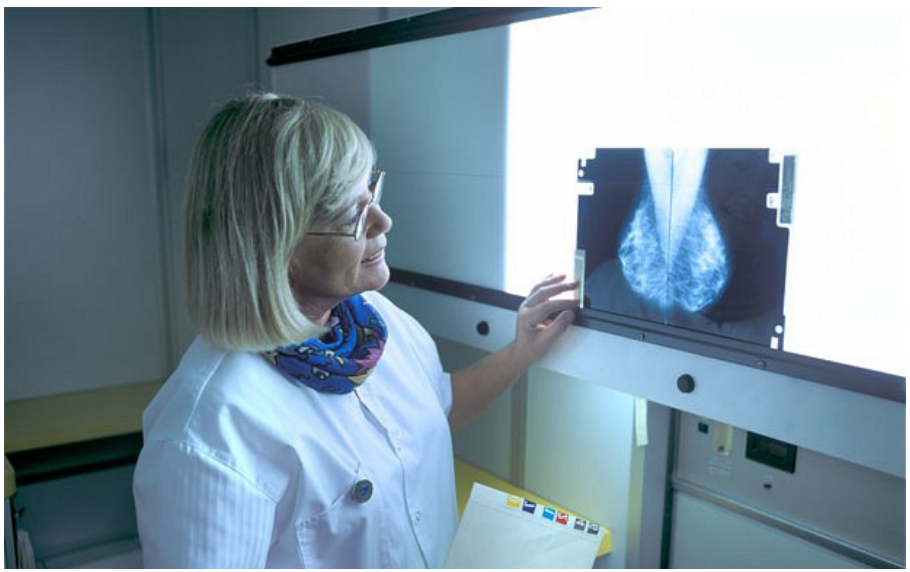

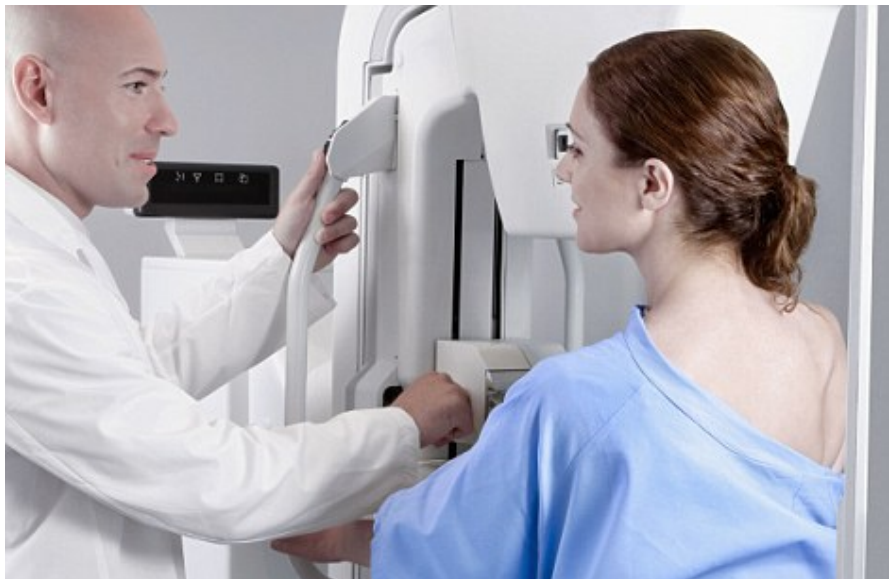

Example: Wisconsin Breast Cancer

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Sample code	Thickness	Unif. Cell Size	Unif. Cell Shape	Marginal Adhesion	Epithelial Cell Size	Bare Nuclei	Bland Chromatin	Normal Nucleoli	Mitoses	Class
1000025	5	1	1	1	2	1	3	1	1	Benign
1002945	5	4	4	5	7	10	3	2	1	Benign
1015425	3	1	1	1	2	2	3	1	1	Benign
1016277	6	8	8	1	3	4	3	7	1	Benign
1017023	4	1	1	3	2	1	3	1	1	Benign
1017122	8	10	10	8	7	10	9	7	1	Malignant
1018099	1	1	1	1	2	10	3	1	1	Benign
1018561	2	1	2	1	2	1	3	1	1	Benign
1033078	2	1	1	1	2	1	1	1	5	Benign
1033078	4	2	1	1	2	1	2	1	1	Benign
1035283	1	1	1	1	1	1	3	1	1	Benign
1036172	2	1	1	1	2	1	2	1	1	Benign
1041801	5	3	3	3	2	3	4	4	1	Malignant
1043999	1	1	1	1	2	3	3	1	1	Benign
1044572	8	7	5	10	7	9	5	5	4	Malignant
1047630	7	4	6	4	6	1	4	3	1	Malignant
1048672	4	1	1	1	2	1	2	1	1	Benign
1049815	4	1	1	1	2	1	3	1	1	Benign
1050670	10	7	7	6	4	10	4	1	2	Malignant
1050718	6	1	1	1	2	1	3	1	1	Benign
1054590	7	3	2	10	5	10	5	4	4	Malignant
1054593	10	5	5	3	6	7	7	10	1	Malignant
1056784	3	1	1	1	2	1	2	1	1	Benign
1057013	8	4	5	1	2	?	7	3	1	Malignant
1059552	1	1	1	1	2	1	3	1	1	Benign
1065726	5	2	3	4	2	7	3	6	1	Malignant
1066373	3	2	1	1	1	1	2	1	1	Benign
1066979	5	1	1	1	2	1	2	1	1	Benign
1067444	2	1	1	1	2	1	2	1	1	Benign
1070935	1	1	3	1	2	1	1	1	1	Benign
1070935	3	1	1	1	1	1	2	1	1	Benign
1071760	2	1	1	1	2	1	3	1	1	Benign
1072179	10	7	7	3	8	5	7	4	3	Malignant

683 patients, 2×10^9 possible configurations

Categorical Latent Gaussian Process

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We define our model as

Continuous latent space of patients $\mathbf{x}_n \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma_x^2 I)$

Dist. over K dim. functions generating weights $\mathbf{f}_d \sim \mathrm{GP}(\cdot)$

$y_{nd} \overset{\text{iid}}{\sim} \mathrm{Softmax}(\mathbf{f}_d(\mathbf{x}_n))$ test result

$\mathbf{y}_n = (y_{n1}, \ldots, y_{nD})$ medical assessment

N patients $\mathbf{x}_n$, D categorical tests, each with K possible test results

Sparse Gaussian Processes

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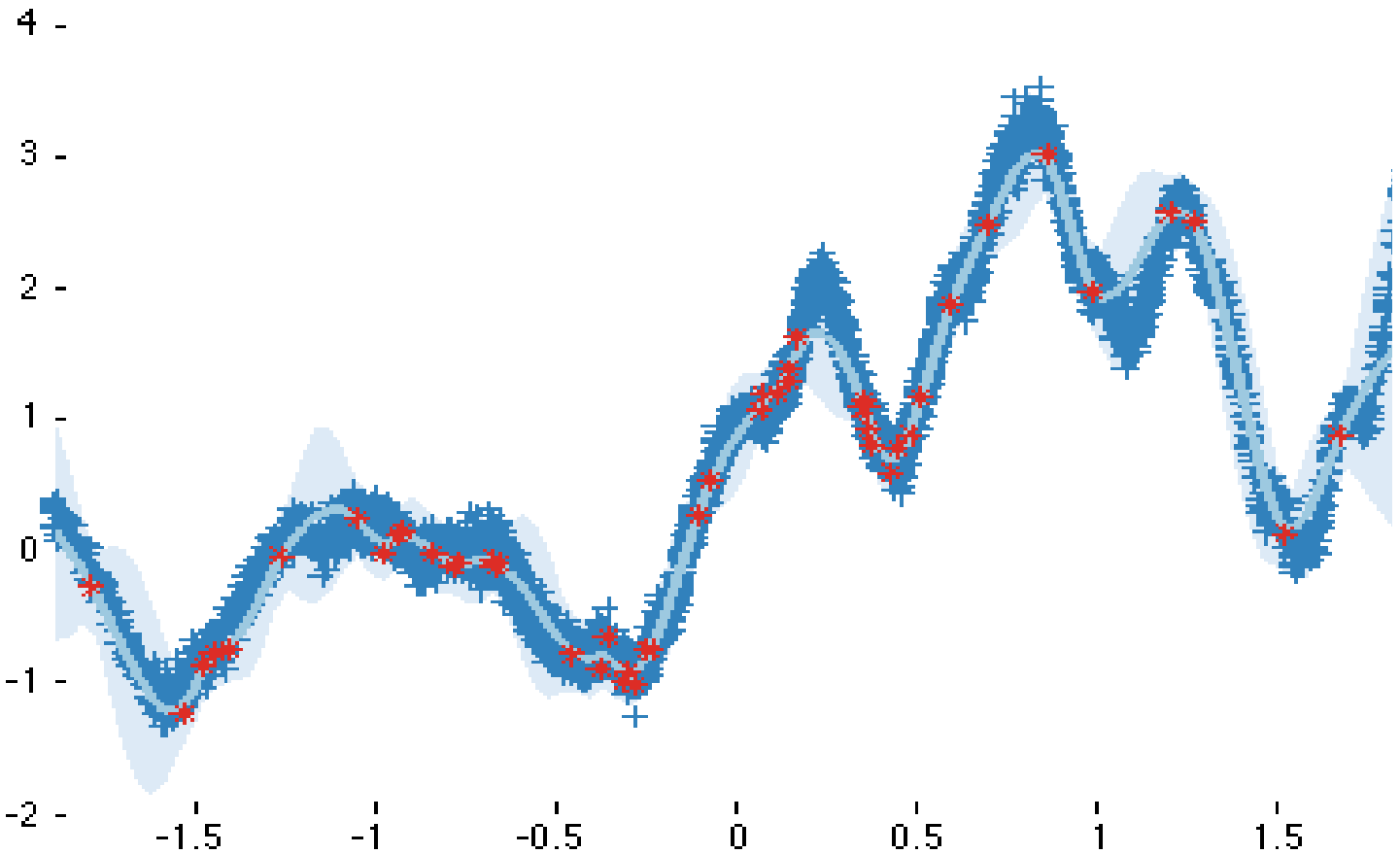
- A small number of inducing points support a distribution over functions



- In dark blue are the data points, in red are the inducing points

Sparse Gaussian Processes

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- Given sufficient statistics $\{Z_m, u_m\}_{m=1}^M$,
  - Define K_{MM} as the kernel evaluated at points (Z_m),
  - Define $K_{Mn} = K_{nM}^T$ as the kernel evaluated between points (Z_m) and point $\mathbf{x}_n$,
- A sparse Gaussian process is defined through a conditional Gaussian distribution by

$$f_n \sim \mathcal{N}(\mathbf{a}_n^T \mathbf{u}, b_n)$$

with

$$\mathbf{a}_n = \mathbf{K}_{MM}^{-1} \mathbf{K}_{Mn}, \quad b_n = K_{nn} - \mathbf{K}_{nM} \mathbf{K}_{MM}^{-1} \mathbf{K}_{Mn},$$

- or equivalently,

$$f_n = \mathbf{a}_n^T \mathbf{u} + \sqrt{b_n} \varepsilon_n^{(f)} \qquad \varepsilon_n^{(f)} \sim \mathcal{N}(0, 1).$$

Generative Model

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- The resulting generative model, with kernel $\mathbf{K}(\cdot,\cdot)$, is

$$
\begin{aligned}
\mathbf{x}_n &\overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma_x^2 I) && \text{patient } n \\
(\mathbf{u}_{dk})_{k=1}^{K} &\sim \mathrm{GP}(0, \mathbf{K}((Z_m)_{m=1}^{M})) && \text{inducing points} \\
f_{ndk} | \mathbf{x}_n, \mathbf{u}_{dk} &\sim \mathcal{N}(\mathbf{a}_n^T \mathbf{u}_{dk}, b_n) && \text{weight of test result } k \\
y_{nd} &\overset{\text{iid}}{\sim} \mathrm{Softmax}(f_{nd1}, \ldots, f_{ndK}) && \text{examination } d \\
\mathbf{y}_n &= (y_{n1}, \ldots, y_{nD}) && \text{medical assessment}
\end{aligned}
$$

- We want to find the posterior over $\mathbf{X}$ and $\mathbf{U}$:

$$p(\mathbf{X}, \mathbf{U} | \mathbf{Y}).$$

- Our marginal log-likelihood is intractable.
- We lower bound the log evidence with a variational approximate posterior $q(\mathbf{X}, \mathbf{F}, \mathbf{U}) = q(\mathbf{X})q(\mathbf{U})p(\mathbf{F}|\mathbf{X}, \mathbf{U})$, with

$$q(\mathbf{X}) = \prod_{n=1}^{N} \prod_{i=1}^{Q} \mathcal{N}(x_{ni}|m_{ni}, s_{ni}^2),$$

$$q(\mathbf{U}) = \prod_{d=1}^{D} \prod_{k=1}^{K} \mathcal{N}(\mathbf{u}_{dk}|\boldsymbol{\mu}_{dk}, L_d L_d^T)$$

- Such that...

$$q(\mathbf{X}, \mathbf{F}, \mathbf{U}) \approx p(\mathbf{X}, \mathbf{F}, \mathbf{U}|\mathbf{Y}).$$

Re-parametrising the Model

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This is equivalent to...

$$x_{ni} = m_{ni} + s_{ni}\varepsilon_{ni}^{(x)} \qquad \varepsilon_{ni}^{(x)} \sim \mathcal{N}(0,1)$$
$$\mathbf{u}_{dk} = \boldsymbol{\mu}_{dk} + \mathbf{L}_d\boldsymbol{\varepsilon}_{dk}^{(u)} \qquad \boldsymbol{\varepsilon}_{dk}^{(u)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_M)$$
$$f_{ndk} = \mathbf{a}_n^T\mathbf{u}_{dk} + \sqrt{b_n}\varepsilon_{ndk}^{(f)} \qquad \varepsilon_{ndk}^{(f)} \sim \mathcal{N}(0,1)$$

Then,

$$\log p(\mathbf{Y}) \geq -\text{KL divergence terms}$$
$$+\sum_{n=1}^{N}\sum_{d=1}^{D}\mathbb{E}_{\varepsilon_n^{(x)},\varepsilon_d^{(u)},\varepsilon_{nd}^{(f)}}\Bigg[$$
$$\log \text{Softmax}\left(\mathbf{y}_{nd}\middle|\mathbf{f}_{nd}\left(\varepsilon_{nd}^{(f)}, \mathbf{U}_d(\varepsilon_d^{(u)}), \mathbf{x}_n(\varepsilon_n^{(x)})\right)\right)\Bigg].$$

Monte Carlo integration

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- Monte Carlo integration approximates the likelihood obtaining noisy gradients:

$$\mathbb{E}_{\varepsilon_n^{(x)},\varepsilon_d^{(u)},\varepsilon_{nd}^{(f)}} \log \text{Softmax}\left(\cdot\right)$$
$$\approx \frac{1}{T}\sum_{i=1}^{T} \log \text{Softmax}\left(\mathbf{y}_{nd}\middle|\mathbf{f}_{nd}\left(\varepsilon_{nd,i}^{(f)}, \mathbf{U}_d(\varepsilon_{d,i}^{(u)}), \mathbf{x}_n(\varepsilon_{n,i}^{(x)})\right)\right)$$

  with $\varepsilon_{\cdot,i}^{(x)}, \varepsilon_{\cdot,i}^{(u)}, \varepsilon_{\cdot,i}^{(f)} \sim \mathcal{N}(0,1)$, independent of the parameters.
- Adaptive learning-rate stochastic optimisation is used to optimise the noisy objective wrt the parameters of the variational distribution.

Categorical Latent Gaussian Process

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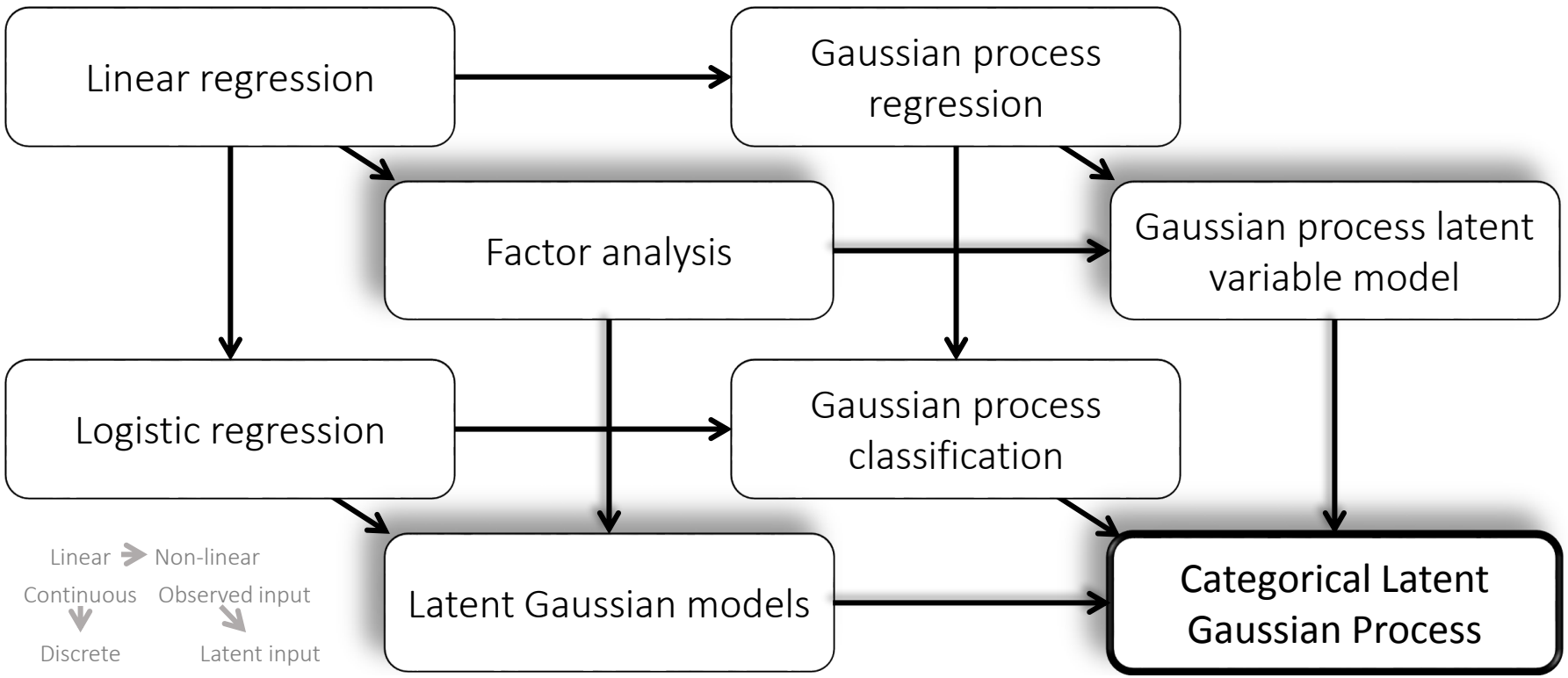
- Symbolic differentiation gives simple code:

```
import theano.tensor as T
X = m + s * randn(N, Q)
U = mu + L.dot(randn(M, K))
Kmm, Kmn, Knn = RBF(sf2, l, Z), RBF(sf2, l, Z, X), RBFnn(sf2, l, X)
KmmInv = sT.matrix_inverse(Kmm)
A = KmmInv.dot(Kmn)
B = Knn - T.sum(Kmn * KmmInv.dot(Kmn), 0)
F = A.T.dot(U) + B[:,None]**0.5 * randn(N, K)
S = T.nnet.softmax(F)
KL_U, KL_X = get_KL_U(), get_KL_X()
LS = T.sum(T.log(T.sum(Y * S, 1))) - KL_U - KL_X
LS_func = theano.function(['''inputs'''], LS)
dLS_dm = theano.function(['''inputs'''], T.grad(LS, m)) # and others
# ... and run RMS-PROP
```

Relations to Existing Models



Multi-modal Distributions

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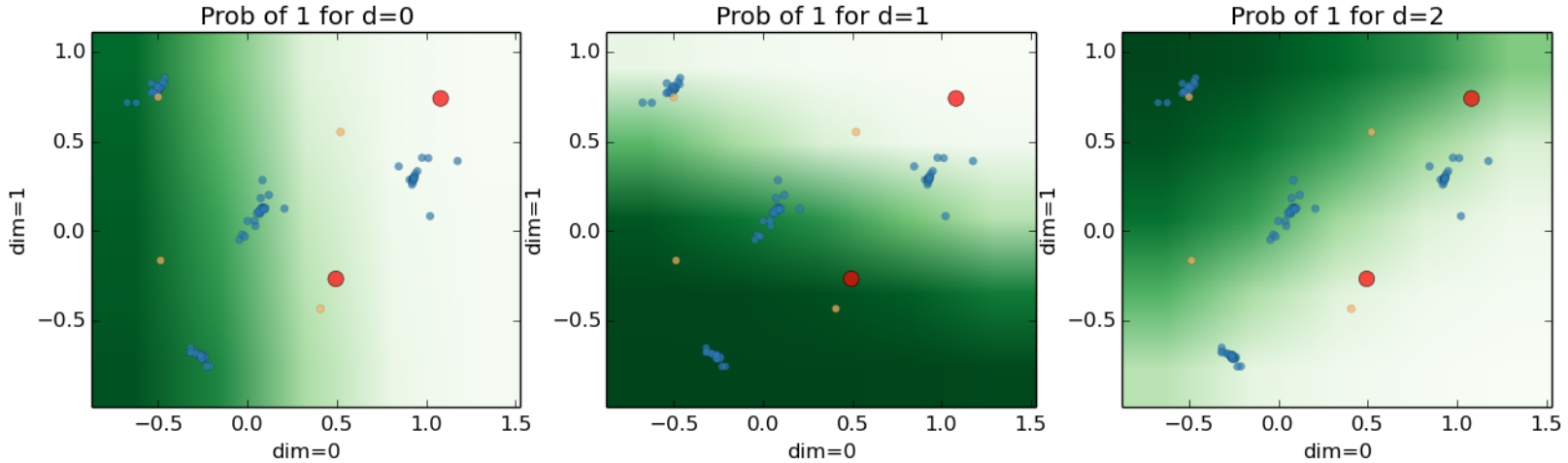
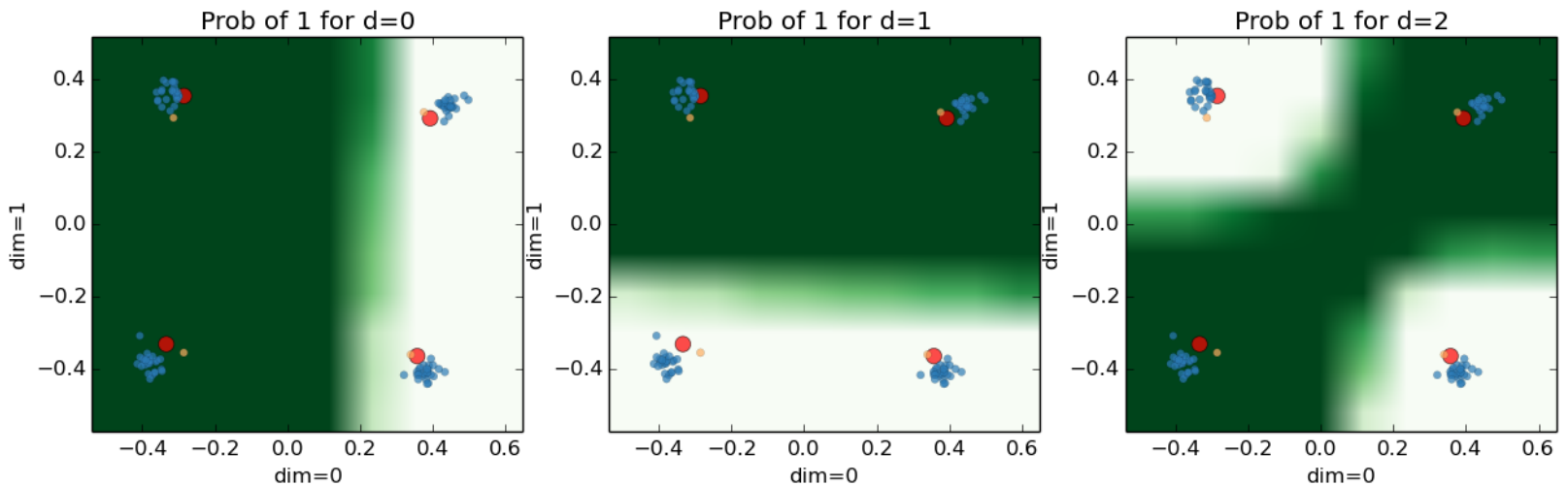


(a) (Linear) Latent Gaussian Model



(b) Categorical Latent Gaussian Process

$p(\mathbf{y}_d = 1|\mathbf{x})$ **as a function of x, for** $d = 0, 1, 2$

(first, second, and third digits in the XOR triplet left to right)

Data Visualisation

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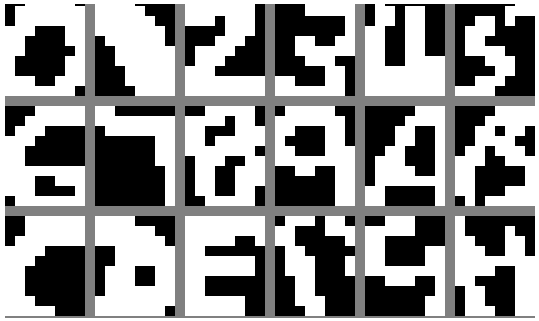
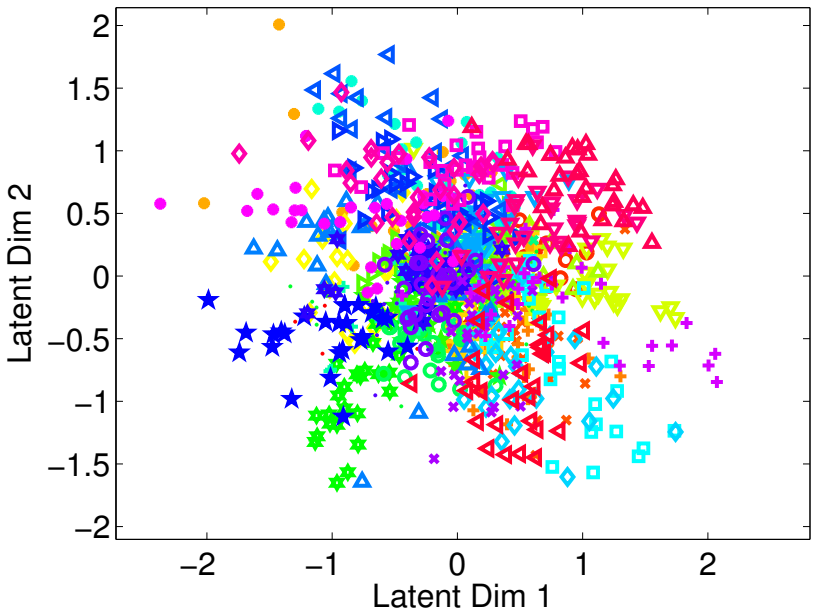
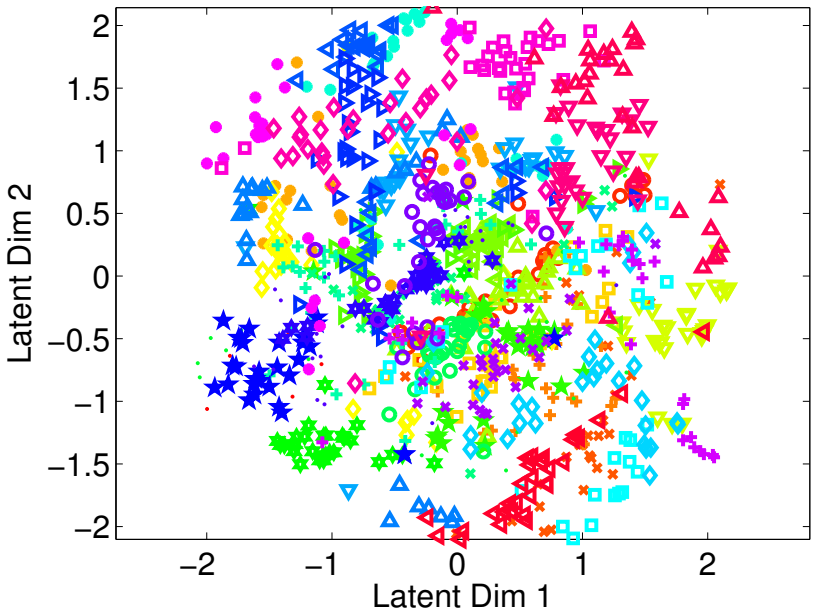


(a) Example alphadigits



(b) (Linear) Latent Gaussian Model latent space



(c) Categorical Latent Gaussian Process latent space

Data Imputation

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Terror Warning Effects on Political Attitude (START Terrorism Data Archive - 17 categorical variables with 5-6 values)

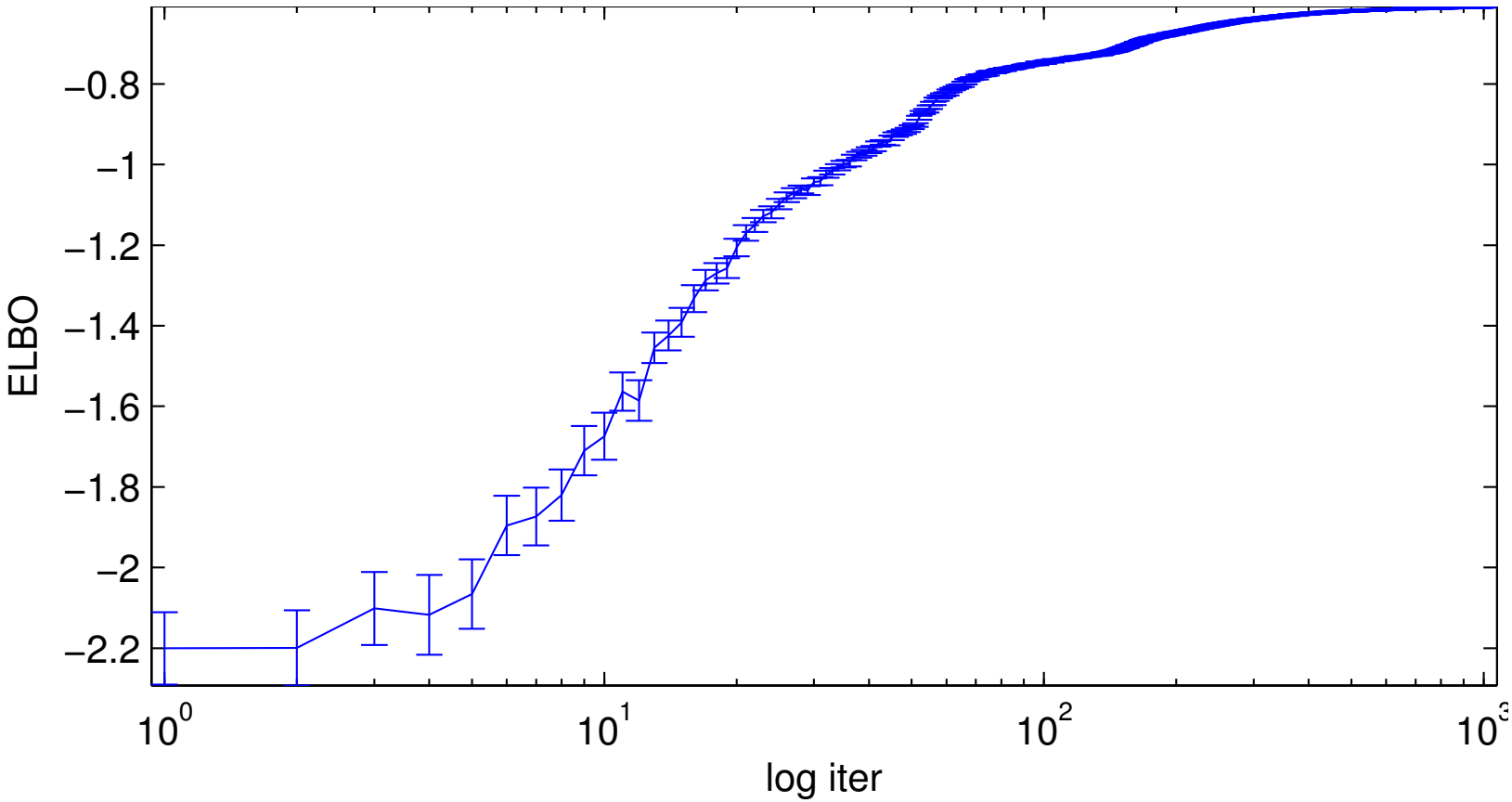
Uniform	Multinomial	(Linear) Latent Gaussian Model	**Categorical Latent Gaussian Process**
2.50	2.20	3.07	**2.11**

Wisconsin Breast cancer (9 categorical variables with 10 values)

Uniform	Multinomial	(Linear) Latent Gaussian Model	**Categorical Latent Gaussian Process**
8.68	4.41	3.57 ± 0.208	$\mathbf{2.86 \pm 0.119}$

Test perplexity predicting randomly missing values

Inference Robustness



Lower bound and MC standard deviation per iteration (on log scale) for the Alphadigits dataset.

Scaling Up!

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- Why not scale the model up?
  - We recently showed that sparse Gaussian processes can be scaled well to millions of data points [Gal, van der Wilk, Rasmussen, 2014]
  - Mini-batch GP optimisation [Hensman el at. 2014]
- Recognition models with sparse Gaussian processes
  - Integrate over unobserved variables
  - Handle missing data
- Mixed data
  - Using link functions alternative to the Softmax
  - Continuous variables, Positives, Ordinals

Currently running experiments!

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Thank you

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