Additive Kernel GPPVAE

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Motivation for the work

- Variational Autoencoders (VAE) are a powerful method for unsupervised learning
- However the i.i.d. assumption for latent representations is too strong
- We would like to include label covariates, such as time, in the model
- Multiple extensions and variations on the VAE have been published
- ...

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- Gaussian Process Variational Autoencoder (GPPVAE) is one such extension
- Gaussian Processes (GPs) act as prior for the latent space
- The GPs are indexed with label information
- Once the model is trained, we can perform label inference on new data

Bayesian inference

- In a generative model the probability of observations is defined by a likelihood $p(x|z)$ and prior on the latent space $p(z)$
- Ideally we could simply maximize the marginal probability of the posterior

$$p(z \mid x) = \frac{p(x \mid z)p(z)}{p(x)}$$

- However, the evidence term in the denominator is intractable
- Therefore we use a variational approximation where the latent distribution and the likelihoods are parametrized by NNs

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Structure of a VAE

- We optimize the variational approximation of the latent distribution by minimizing the KL divergence between it, and the prior
- This is equivalent to maximizing the evidence lower bound, or ELBO

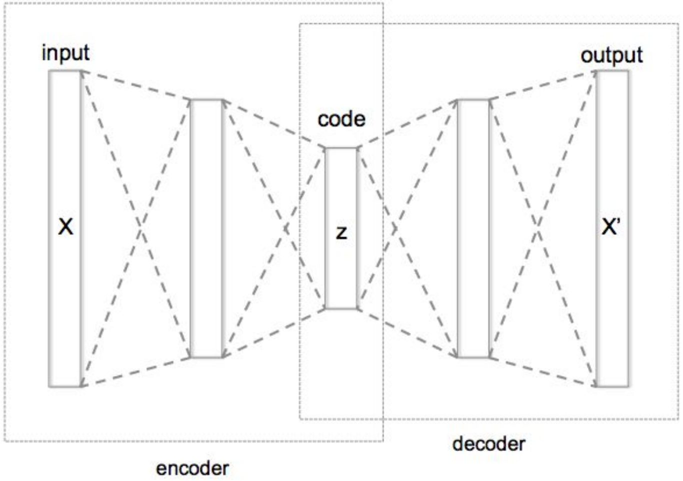

Figure from Wikipedia

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(Very) short intro to Gaussian Processes

- A Gaussian process is a stochastic process where each finite collection of variables has a multivariate normal distribution
- A zero mean GP is completely defined by its covariance function, or kernel
- The choice of kernel defines the function space in GP regression

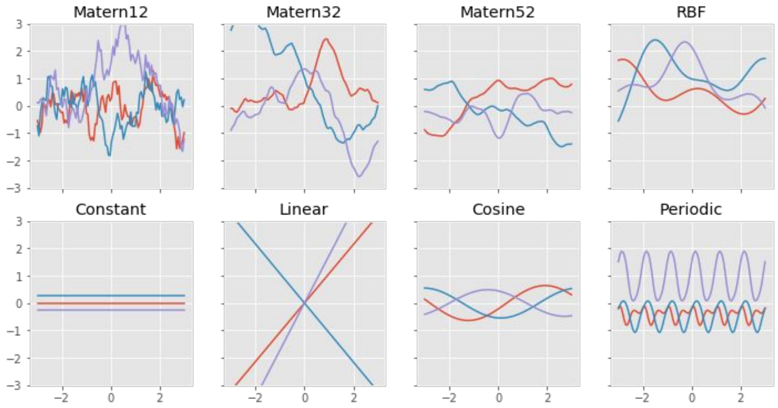

Figure from GPflow by Matthews et al.

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Gaussian prior

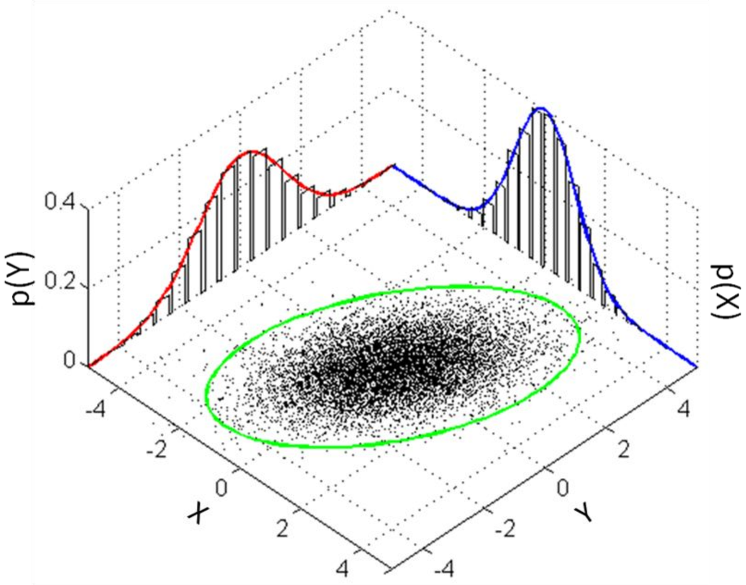

Figure from Wikipedia

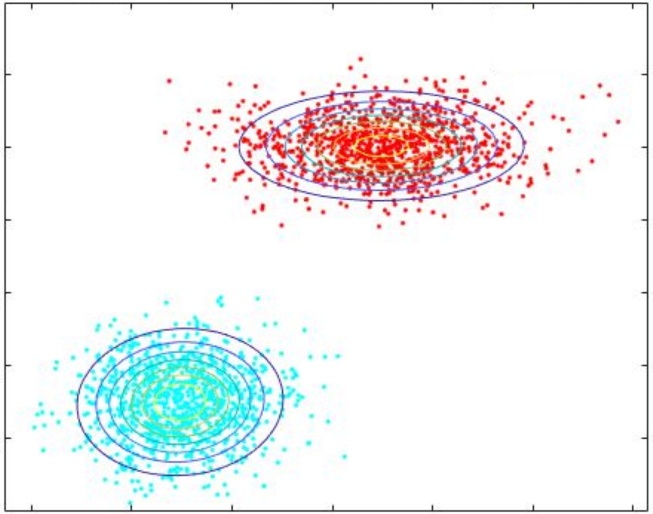

Figure by MathWorks

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ELBO for GPPVAE

- ELBO derived by Casale et al.

$$\log p(\boldsymbol{Y} \mid \boldsymbol{X}, \boldsymbol{W}, \phi, \sigma_y^2, \boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z} \sim q_{\psi}} \left[\sum_n \log \mathcal{N}(\boldsymbol{y}_n \mid g_{\boldsymbol{\phi}}(\boldsymbol{z}_n), \sigma_y^2 \boldsymbol{I}_K) + \log p(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{W}, \boldsymbol{\theta}, \alpha) \right] + \\ + \frac{1}{2} \sum_{nl} \log(\boldsymbol{\sigma}^{z}{}_{\boldsymbol{\psi}}^{2}(\boldsymbol{y}_n)_l) + \text{const.}$$

- Which gives the loss for SGD

$$l(\boldsymbol{\phi}, \boldsymbol{\psi}, \boldsymbol{\theta}, \alpha, \sigma_y^2) = \\ = NK \log \sigma_y^2 + \underbrace{\sum_n \frac{\left\| \boldsymbol{y}_n - g_{\boldsymbol{\phi}}(\boldsymbol{z}_{\boldsymbol{\psi}_n}) \right\|^2}{2\sigma_y^2}}_{\text{reconstruction term}} - \underbrace{\log p(\boldsymbol{Z}_{\boldsymbol{\psi}} \mid \boldsymbol{X}, \boldsymbol{W}, \boldsymbol{\theta}, \alpha)}_{\text{latent-space GP term}} + \underbrace{\frac{1}{2} \sum_{nl} \log(\boldsymbol{\sigma}^{z}{}_{\boldsymbol{\psi}}^{2}(\boldsymbol{y}_n)_l)}_{\text{regularization term}},$$

GP likelihoods

The marginal likelihood for observations

$$p(\boldsymbol{y}, f_*) = \int p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}, f_*)\mathrm{d}\boldsymbol{f}$$
$$= \mathcal{N}\left(\begin{bmatrix} \boldsymbol{y} \\ f_* \end{bmatrix} \middle| \boldsymbol{0}, \begin{bmatrix} \boldsymbol{K}_{ff} + \sigma^2\boldsymbol{I} & \boldsymbol{K}_{f_* f} \\ \boldsymbol{K}_{f_* f} & K_{f_* f_*} \end{bmatrix}\right)$$

The marginal likelihood of kernel parameters

$$p(\boldsymbol{y}|\boldsymbol{\theta}) = \int p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}|\boldsymbol{\theta})\mathrm{d}\boldsymbol{f}$$
$$= \int \mathcal{N}\left(\boldsymbol{y}|\boldsymbol{f}, \sigma^2\boldsymbol{I}\right)\mathcal{N}\left(\boldsymbol{f}|\boldsymbol{0}, \boldsymbol{K}\right)\mathrm{d}\boldsymbol{f}$$
$$= \mathcal{N}\left(\boldsymbol{y}|\boldsymbol{0}, \sigma^2\boldsymbol{I} + \boldsymbol{K}\right)$$

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Additive and multiplicative kernels

- It would be most beneficial if kernels could be configured in a modular and flexible manner
- My implementations allows for kernel addition and multiplication thanks to the GPyTorch library

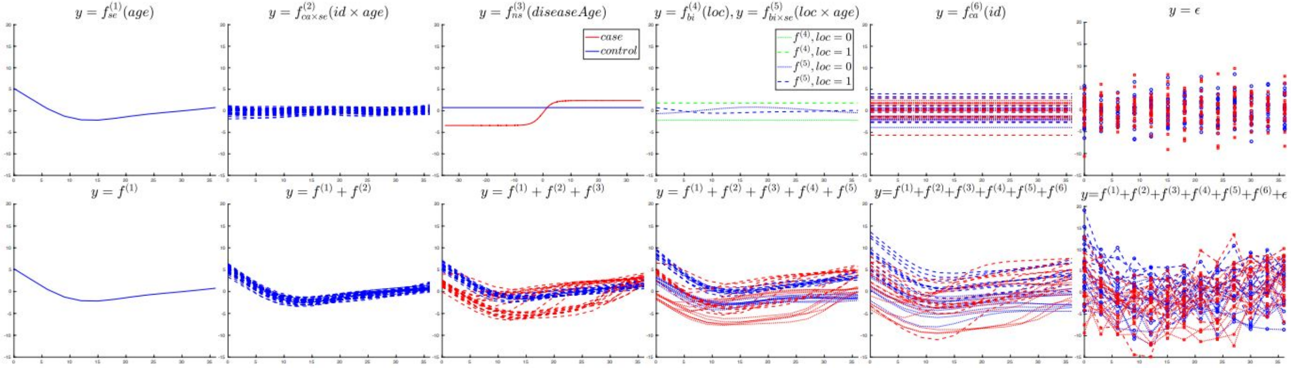

Figure by Cheng et al.

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Software Implementation

- The implementation was built using PyTorch and the GPyTorch GP library
- GPyTorch provides a highly modular and flexible framework for building GP models, which can be modified to suit specific requirements
- The implementation is available at Aalto Version

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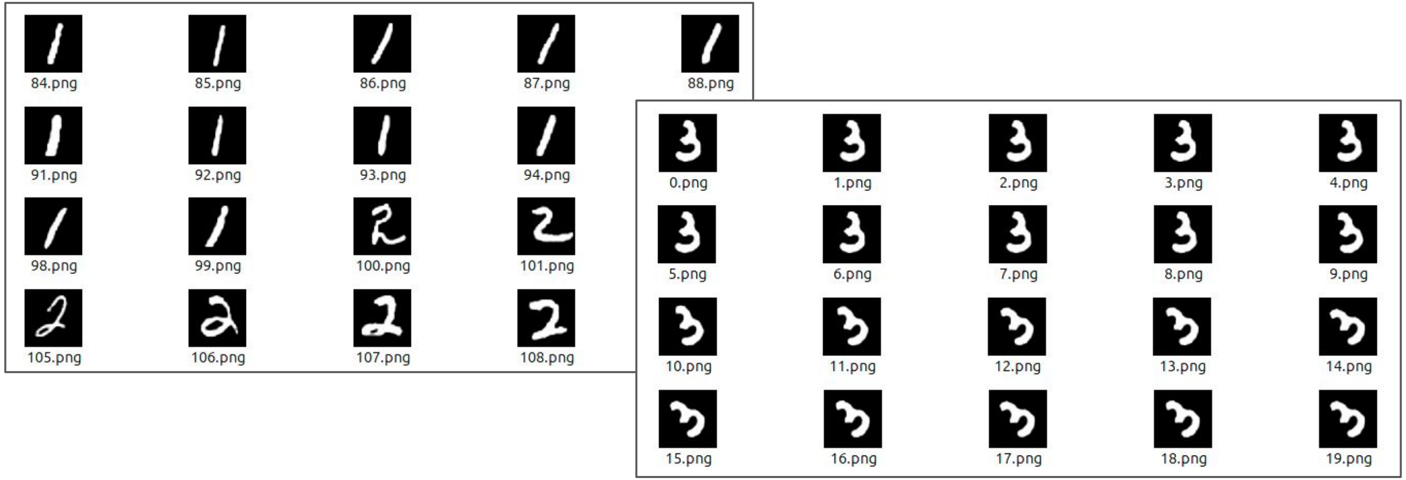
Test datasets

- The implementation was tested using two toy datasets



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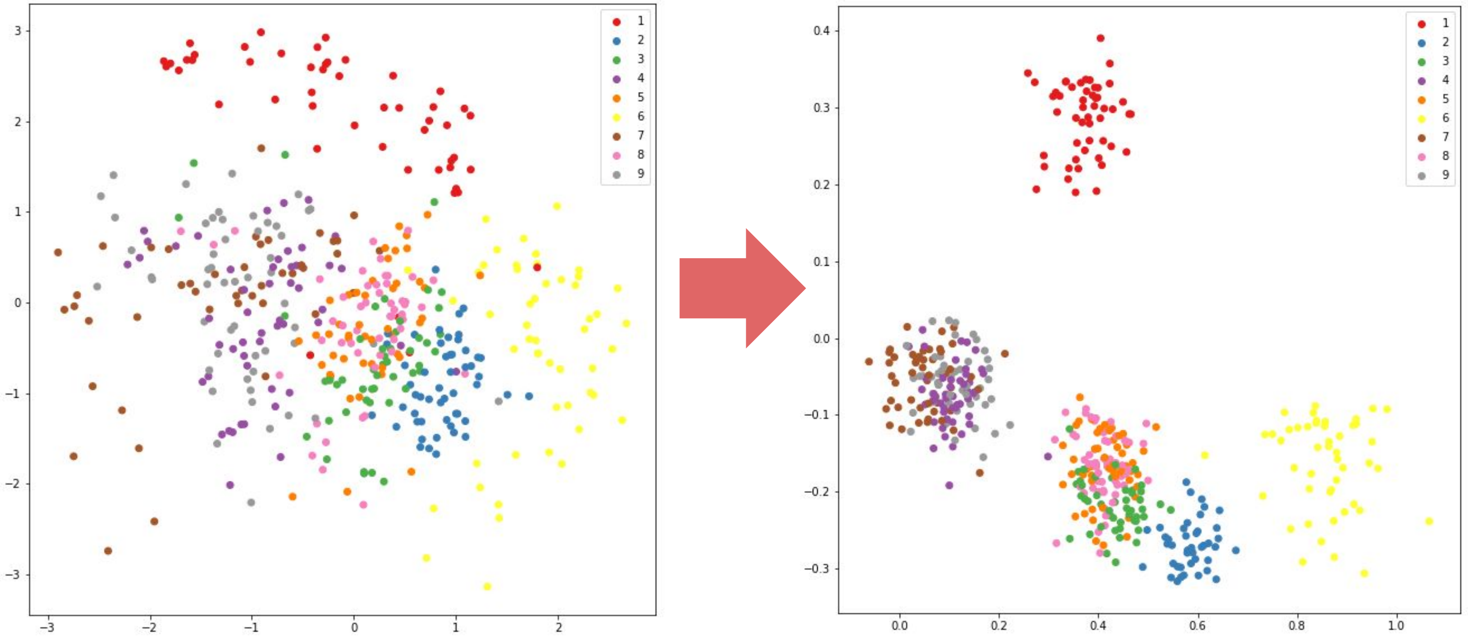
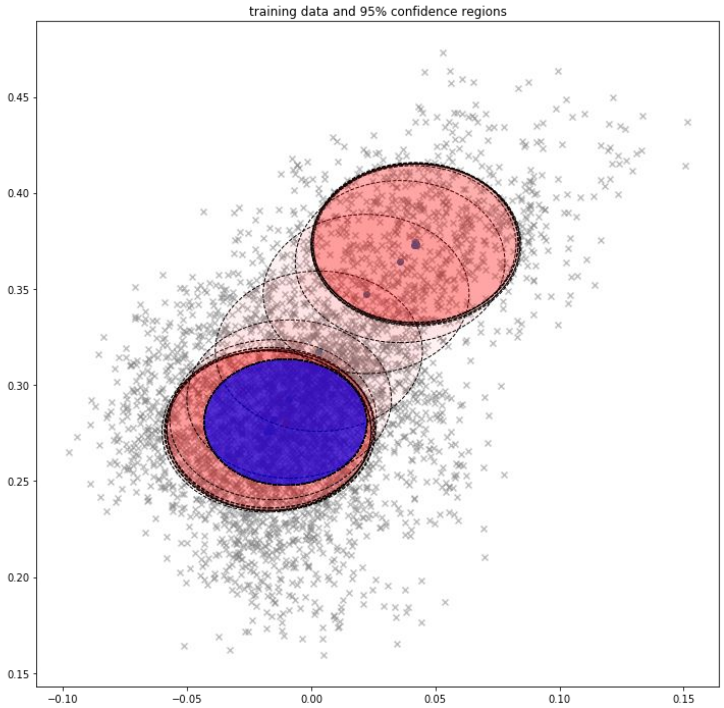
MNIST with categorical kernel



Rotating MNIST with binary + warping kernel



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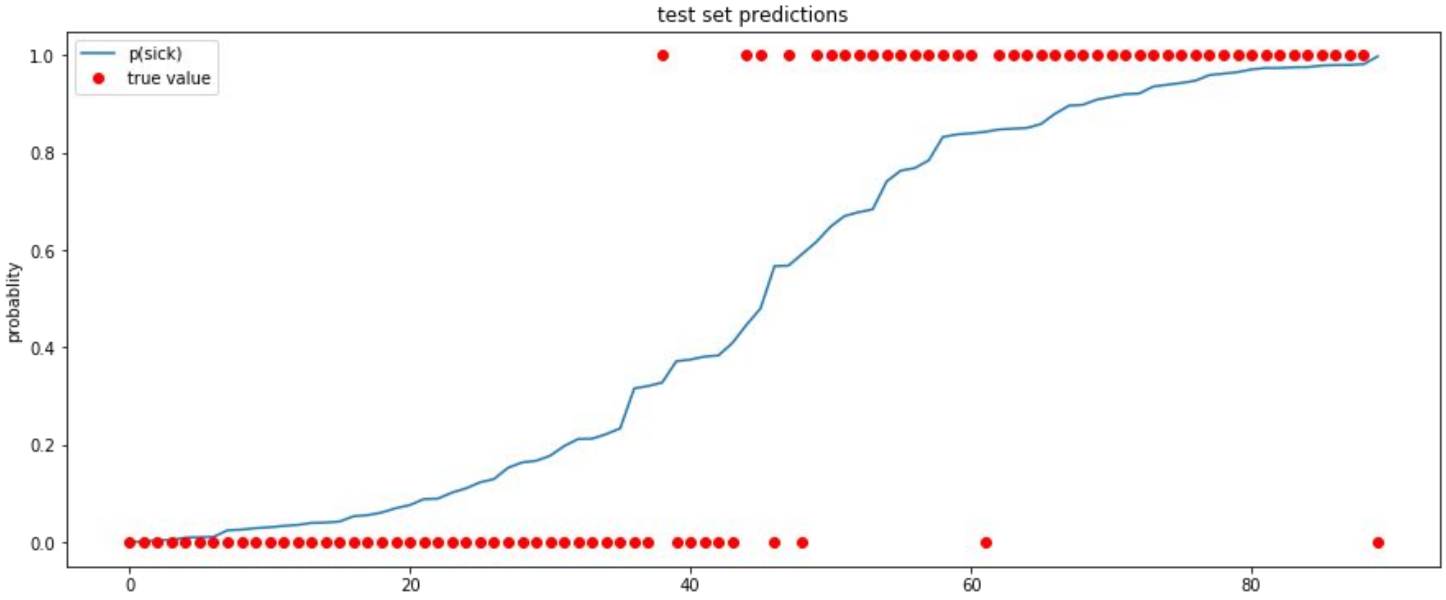
Rotating MNIST label inference



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All code and notebooks available at:

https://version.aalto.fi/gitlab/mentus1/HIT_VAE

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Special thanks to Gleb Tikhonov

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