# Scaling Up Deep Gaussian Processes

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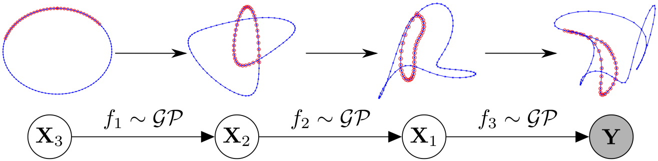
# Deep GPs




$$\mathbf{Y} = f_1(\mathbf{X}_1) + \epsilon_1, \quad \epsilon_1 \sim \mathcal{N}(0, \sigma_1^2 \mathbf{I})$$

$$\mathbf{X}_{l-1} = f_l(\mathbf{X}_l) + \epsilon_l, \quad \epsilon_l \sim \mathcal{N}(0, \sigma_l^2 \mathbf{I}), \quad l = 2 \dots L$$

$$f_l(x) \sim \mathcal{GP}(0, k_l(x, x'))$$

# Motivations

- Represent a complex family of functions with one type of kernels such as RBF.
- Cubic scaling with width, while linear scaling with depth

# Limitations

- Damianou and Lawrence [2013] show the results with a small number of data points.
- The number of variational parameters scales linearly with the size of data.

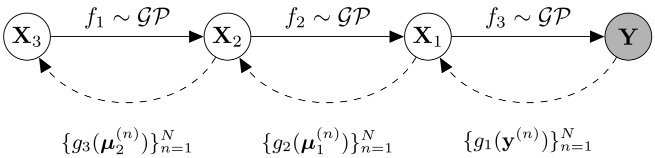
# Parallelization / GPU

- Parallelization of Bayesian GPLVM and Sparse GP ([Gal et al., 2014, Dai et al., 2014])
- Go towards millions of data points
- Deep GPs

# Variational Auto-Encoder / Back-constrained GP

- [Lawrence and Quiñonero-Candela, 2006]
- [Kingma and Welling, 2013]

# Variational Auto-encoder in DGP

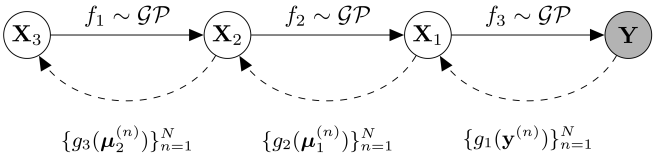



- Mean-field approximation for $\mathbf{X}$: $q(\mathbf{X}) = q(\mathbf{X}_1)q(\mathbf{X}_2)q(\mathbf{X}_3)$
- Assume Gaussian distribution:

$$q(\mathbf{X}_1) = \prod_{n=1}^{N} \mathcal{N}(\mathbf{x}_1^{(n)} | \boldsymbol{\mu}_1^{(n)}, \Sigma_1)$$

- Reparameterization of variational posteriors: $\boldsymbol{\mu}_1^{(n)} = g_1(\mathbf{y}^{(n)})$, $\boldsymbol{\mu}_2^{(n)} = g_2(\boldsymbol{\mu}_1^{(n)})$, $\boldsymbol{\mu}_3^{(n)} = g_3(\boldsymbol{\mu}_2^{(n)})$
- Deterministic transformations: $\boldsymbol{\mu}_l^{(n)} = g_l(\ldots g_1(\mathbf{y}^{(n)}))$.

# Variational Auto-encoder in DGP




The choice of $\Sigma_1$?

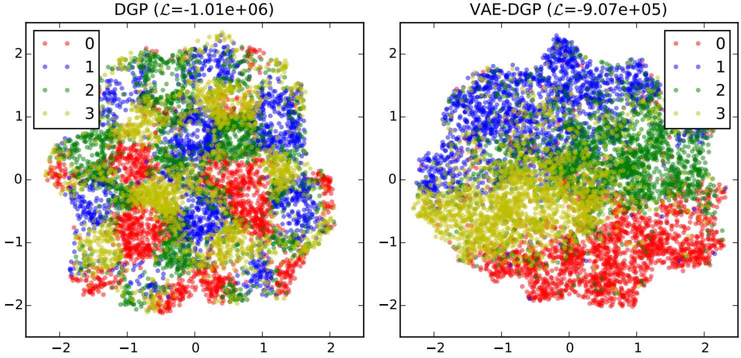
- constant for all the data points (our choice)
- $(\Sigma_1^{(n)})_{ii} = \exp\left(h_{1i}(\mathbf{y}^{(n)})\right)$
- Normalizing flow [Rezende and Mohamed, 2015]
- Variational GP [Tran et al., 2016]

# Benefits: Avoid Local Optima

Unsupervised Learning with the *Same Initialization*

one layer with 2D latent space (Bayesian GPLVM)

10,000 noisy MNIST digits (0,1,2,3)



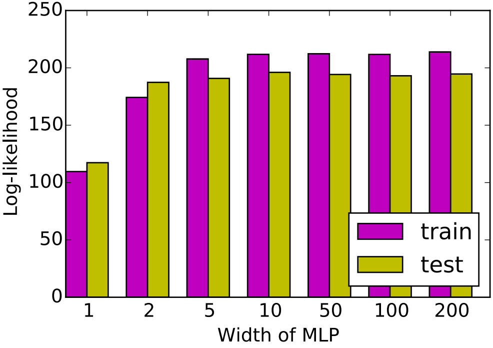

https://youtu.be/4IryFhMYvn4

# Benefits: Recognition Model does not Overfit

Unsupervised Learning with varying the size of recognition model

one layer with 2D latent space (Bayesian GPLVM)

2,000 MNIST digit ‘0’



# Parallelization of Deep GPs

The marginal likelihood for two hidden layer model:

$$p(\mathbf{Y}) = \int p(\mathbf{Y}|\mathbf{X}_1)p(\mathbf{X}_1|\mathbf{X}_2)p(\mathbf{X}_2)\mathsf{d}\mathbf{X}_1\mathsf{d}\mathbf{X}_2$$

The variational lower bound:

$$\begin{aligned}\log p(\mathbf{Y}) \geq & \int q(\mathbf{X}_1)q(\mathbf{X}_2)\log\frac{p(\mathbf{Y}|\mathbf{X}_1)p(\mathbf{X}_1|\mathbf{X}_2)p(\mathbf{X}_2)}{q(\mathbf{X}_1)q(\mathbf{X}_2)}\mathsf{d}\mathbf{X}_1\mathsf{d}\mathbf{X}_2 \\ = & \left\langle p(\mathbf{Y}|\mathbf{X}_1)\right\rangle_{q(\mathbf{X}_1)} + \left\langle p(\mathbf{X}_1|\mathbf{X}_2)\right\rangle_{q(\mathbf{X}_2)} + H(q(\mathbf{X}_1)) \\ & - \mathsf{KL}\left(q(\mathbf{X}_2)\,\|\,p(\mathbf{X}_2)\right)\end{aligned}$$

# Parallelization of Deep GPs

$p(\mathbf{Y}|\mathbf{X}_1)$ and $p(\mathbf{X}_1|\mathbf{X}_2)$ are both GPs.
With the sparse GP formulation and Gaussian likelihood distribution:

$$p(\mathbf{Y}|\mathbf{X}_1) = \int p(\mathbf{Y}|\mathbf{F}_1)p(\mathbf{F}_1|\mathbf{U}_1, \mathbf{X}_1)p(\mathbf{U}_1)\mathrm{d}\mathbf{F}_1\mathrm{d}\mathbf{U}_1,$$

With the variational approximation:
$q(\mathbf{F}_1, \mathbf{U}_1|\mathbf{X}_1) = p(\mathbf{F}_1|\mathbf{U}_1, \mathbf{X}_1)q(\mathbf{U}_1)$

$$\begin{aligned}\langle p(\mathbf{Y}|\mathbf{X}_1)\rangle_{q(\mathbf{X}_1)} \geq \langle \log p(\mathbf{Y}|\mathbf{F}_1)\rangle_{p(\mathbf{F}_1|\mathbf{U}_1,\mathbf{X}_1)q(\mathbf{U}_1)q(\mathbf{X}_1)} \\ - \mathsf{KL}\left(q(\mathbf{U}_1) \,\|\, p(\mathbf{U}_1)\right)\end{aligned}$$

# Parallelization of Deep GPs

Gal et al. [2014], Dai et al. [2014] show the computation can be parallelized following *data parallelism*.

$$\mathrm{Tr}(\mathbf{Y}^\top \mathbf{Y}) = \sum_{n=1}^{N} (\mathbf{y}^{(n)})^\top \mathbf{y}^{(n)},$$

$$\mathrm{Tr}(\mathbf{\Lambda}_1^{-1} \mathbf{\Psi}_1^\top \mathbf{Y}\mathbf{Y}^\top \mathbf{\Psi}_1) = \mathrm{Tr}\left( \mathbf{\Lambda}_1^{-1} \left( \sum_{n=1}^{N} \mathbf{\Psi}_1^{(n)} (\mathbf{y}^{(n)})^\top \right) \left( \sum_{n=1}^{N} \mathbf{\Psi}_1^{(n)} (\mathbf{y}^{(n)})^\top \right)^\top \right),$$

$$\mathbf{\Psi}_1 = \left\langle \mathbf{K}_{\mathbf{F}_1\mathbf{U}_1} \right\rangle_{q(\mathbf{X}_1)}, \ \mathbf{\Phi}_1 = \left\langle \mathbf{K}_{\mathbf{F}_1\mathbf{U}_1}^\top \mathbf{K}_{\mathbf{F}_1\mathbf{U}_1} \right\rangle_{q(\mathbf{X}_1)},$$

$$\mathbf{\Lambda}_1 = \mathbf{K}_{\mathbf{U}_1\mathbf{U}_1} + \mathbf{\Phi}_1$$

# Parallelization of Deep GPs

In deep GPs, $p(\mathbf{X}_1|\mathbf{X}_2)$ leads to the computation of $\mathrm{Tr}(\left\langle \mathbf{X}_{l-1}^\top \mathbf{X}_{l-1} \right\rangle_{q(\mathbf{X}_{l-1})})$ and $\mathrm{Tr}(\mathbf{\Lambda}_l^{-1} \mathbf{\Psi}_l^\top \left\langle \mathbf{X}_{l-1} \mathbf{X}_{l-1}^\top \right\rangle_{q(\mathbf{X}_{l-1})} \mathbf{\Psi}_l)$.

$$\mathrm{Tr}(\left\langle \mathbf{X}_{l-1}^\top \mathbf{X}_{l-1} \right\rangle_{q(\mathbf{X}_{l-1})}) = \sum_{n=1}^{N} (\boldsymbol{\mu}_{l-1}^{(n)})^\top \boldsymbol{\mu}_{l-1}^{(n)} + \mathrm{Tr}(\mathbf{\Sigma}_{l-1}^{(n)})$$

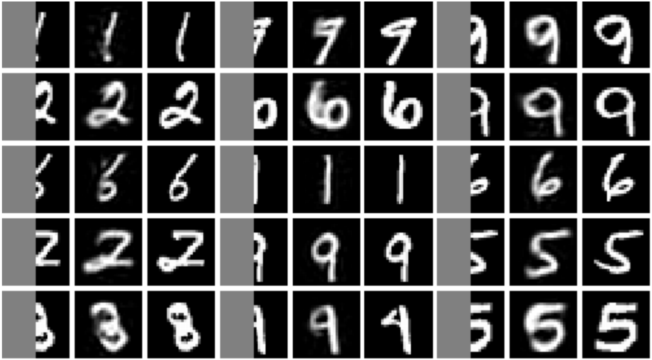
# Parallelization of Deep GPs

For the second term, we can rewrite $\left\langle \mathbf{X}_{l-1}\mathbf{X}_{l-1}^\top \right\rangle_{q(\mathbf{X}_{l-1})} = \mathbf{R}_{l-1}^\top \mathbf{R}_{l-1} + \mathbf{A}_{l-1}\mathbf{A}_{l-1}$, where $\mathbf{R}_{l-1} = [(\boldsymbol{\mu}_{(l-1)}^{(1)})^\top, \ldots, (\boldsymbol{\mu}_{(l-1)}^{(N)})^\top]$, $\mathbf{A}_{l-1} = \mathrm{diag}(\alpha_{l-1}^{(1)}, \ldots, \alpha_{l-1}^{(N)})$ and $\alpha_{l-1}^{(n)} = \mathrm{Tr}(\boldsymbol{\Sigma}_{l-1}^{(n)})^{\frac{1}{2}}$. This enables us to formulate it into a distributable form:

$$\mathrm{Tr}(\boldsymbol{\Lambda}_l^{-1}\boldsymbol{\Psi}_l^\top \left\langle \mathbf{X}_{l-1}\mathbf{X}_{l-1} \right\rangle_{q(\mathbf{X}_{l-1})}^\top \boldsymbol{\Psi}_l) = \mathrm{Tr}\left(\boldsymbol{\Lambda}_l^{-1}\left(\boldsymbol{\Psi}_l^\top \mathbf{R}_{l-1}^\top\right)\left(\mathbf{R}_{l-1}\boldsymbol{\Psi}_l\right)\right)$$
$$+ \mathrm{Tr}\left(\boldsymbol{\Lambda}_l^{-1}\left(\sum_{n=1}^N \boldsymbol{\Psi}_l^{(n)}\alpha_{l-1}^{(n)}\right)\left(\sum_{n=1}^N \boldsymbol{\Psi}_l^{(n)}\alpha_{l-1}^{(n)}\right)^\top\right).$$

# Yale + Frey Faces

# MNIST Imputation



# MNIST Test log-likelihood

| Model | MNIST |
| --- | --- |
| DBN | 138$\pm$2 |
| Stacked CAE | 121 $\pm$ 1.6 |
| Deep GSN | 214 $\pm$ 1.1 |
| Adversarial nets | 225 $\pm$ 2 |
| GMMN+AE | 282 $\pm$ 2 |
| VAE-DGP (5) | 301.67 |
| VAE-DGP (10-50) | 674.86 |
| VAE-DGP (5-20-50) | 723.65 |

# SVHN Imputation

# Future Directions

- Improve the recognition model with a better handling of variance.
- Conditional Variational Posterior $q(\mathbf{X}_2|\mathbf{X}_1)q(\mathbf{X}_1)$ instead of mean-field $q(\mathbf{X}_2)q(\mathbf{X}_1)$
- Stochastic Variational Inference (like [Bui and Turner, 2015])

# Collaborators

- Andreas Damianou
- Javier González
- Neil Lawrence

# References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