Deep Learning for Smoothing in Dynamical Systems

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Outline



Background

Dynamical Systems and State Space Models Filtering and Smoothing Black Box Variational Inference Neural Networks

Implementation

BBVI for Smoothing Using RNN

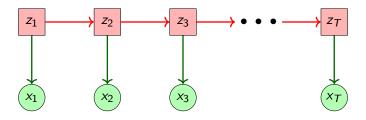
Conclusions



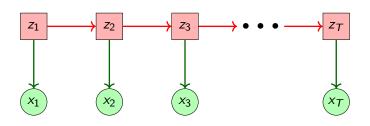
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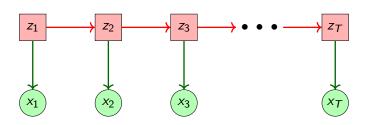






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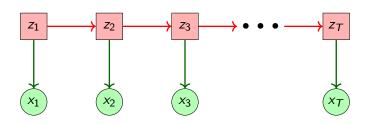




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- \triangleright v_1 and v_2 are noise terms.



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- ▶ if f and g linear and v_1 , v_2 Gaussian white noise the optimal solution is the *Kalman filter/smoother*

Smoothing



▶ Offline problem - finding all z as a function of x

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Smoothing



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- $\mathbf{x} = (x_1, x_2, ..., x_T)$
- $ightharpoonup z = (z_1, z_2, ..., z_T)$

$$p(\mathbf{x},\mathbf{z}) = p(z_0) \Big[\prod_{t=1}^T p(z_t|z_{t-1}) \Big] \Big[\prod_{t=1}^T p(x_t|z_t) \Big]$$



Variational inference



Variational inference

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{x})}$$
 $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$



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- \triangleright $p(\mathbf{x})$ is hard to calculate
- ▶ Idea: use approximate posterior $q_{\theta}(\mathbf{z}|\mathbf{x}) \approx p(\mathbf{z}|\mathbf{x})$



▶ Chose $q_{\theta}(\mathbf{x}|\mathbf{z})$ s.t. it maximises the Evidence Lower Bound (ELBO)

$$\mathcal{L} = \mathbb{E}_{q_{ heta}}[\log p(\mathbf{x}, \mathbf{z})] - \mathbb{E}_{q_{ heta}}[\log q_{ heta}(\mathbf{z}|\mathbf{x})]$$



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 This is equivalent to minimising the Kullback–Leibler divergence

$$D_{\mathsf{KL}}(q||p) = \int_{\Omega} p(\omega) \log \frac{p(\omega)}{q(\omega)} d\omega$$

Black Box Variational Inference



► Still hard to optimise the ELBO

Black Box Variational Inference



- Still hard to optimise the ELBO
- We need the gradient which involves a derivative of an expected value w.r.t. the approximate posterior

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▶ Idea: Sample z from q_θ and calculate noisy gradient

Black Box Variational Inference: Noisy Gradient



Let
$$q_{\theta}(z_t|x_t,...,x_T) = \mathcal{N}(\mu_t, \sigma_t^2)$$

$$z_t = \mu_t + \sigma_t \epsilon =: g_{\theta}(\epsilon)$$

$$\epsilon \sim \mathcal{N}(0,1) =: \rho(\epsilon)$$

Black Box Variational Inference: Noisy Gradient



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 $\epsilon \sim \mathcal{N}(0, 1) =: p(\epsilon)$

Approximate $\nabla_{\theta} \mathcal{L} = \mathbb{E}_{p(\epsilon)}[\nabla f_{\theta}(x, g_{\theta}(\epsilon))] \approx \frac{1}{N} \sum_{i=1}^{N} \nabla f_{\theta}(x, g_{\theta}(\epsilon))$

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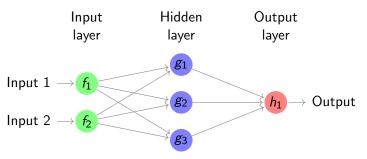
- Approximate $\nabla_{\theta} \mathcal{L} = \mathbb{E}_{p(\epsilon)}[\nabla f_{\theta}(x, g_{\theta}(\epsilon))] \approx \frac{1}{N} \sum_{i=1}^{N} \nabla f_{\theta}(x, g_{\theta}(\epsilon))$
- ▶ This is called the *reparametrisation trick*



▶ A Neural Network is a function of some input variables.



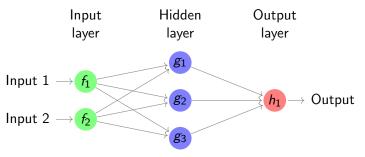
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• A neuron: $g_i(\mathbf{x}) = K(\sum_t \omega_t f_t(\mathbf{x}) + b)$



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- \blacktriangleright b is called a bias and ω is called a weight, K is some non-linear function, called an activation function.



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	Input Iayer	Hidden layer	Output layer	
Input 1 Input 2		g ₁ g ₂ g ₃		Output

- A neuron: $g_i(\mathbf{x}) = K(\sum_t \omega_t f_t(\mathbf{x}) + b)$
- \blacktriangleright b is called a bias and ω is called a weight, K is some non-linear function, called an activation function.
- ► Typically some loss function is minimised w.r.t. the weights and biases.





► State Space Models



- State Space Models
- Smoothing



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- ▶ Black Box Variational Inference



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- Black Box Variational Inference
- ► Neural Networks

Implementation



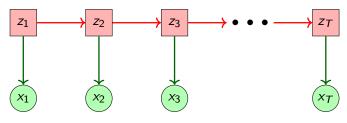
- ► All of the methods here were implemented with Python and TensorFlow.
- TensorFlow is an open source software library commonly used in deep learning.



► RNN: Recurrent neural network, a kind of NN that uses the information from different time steps

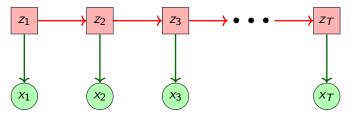


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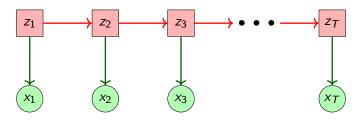


▶ BBVI: Black box variational inference

$$q_{ heta}(\mathbf{z}|\mathbf{x}) \xrightarrow{\mathsf{Optimize}\ heta} \mathsf{Maximize}\ \mathsf{ELBO} \longrightarrow q_{ heta}(\mathbf{z}|\mathbf{x}) pprox p(\mathbf{z}|\mathbf{x})$$



▶ Factorize $q_{\theta}(\mathbf{z}|\mathbf{x})$



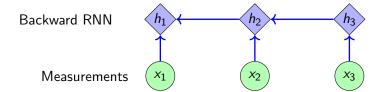
$$\begin{cases} q_{\theta}(\mathbf{z}|\mathbf{x}) = q_{\theta}(z_{1}|x_{1},...,x_{T}) \prod_{t=2}^{T} q_{\theta}(z_{t}|z_{t-1},x_{t},...,x_{T}) \\ q_{\theta}(z_{t}|z_{t-1},x_{t},...,x_{T}) \sim \mathcal{N}(\mu_{t}(z_{t-1},x_{t},...,x_{T}),\sigma_{t}^{2}(z_{t-1},x_{t},...,x_{T})) \end{cases}$$



$$q_{ heta}(\mathbf{z}|\mathbf{x}) = q_{ heta}(z_1|x_1,...,x_T) \prod_{t=2}^T q_{ heta}(z_t|z_{t-1},x_t,...,x_T)$$

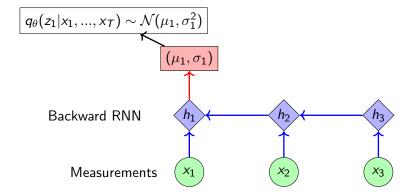


$$q_{\theta}(\mathbf{z}|\mathbf{x}) = q_{\theta}(z_1|x_1,...,x_T) \prod_{t=2}^{I} q_{\theta}(z_t|z_{t-1},x_t,...,x_T)$$

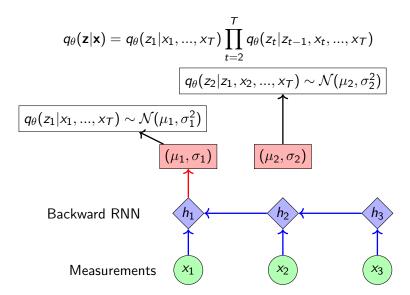




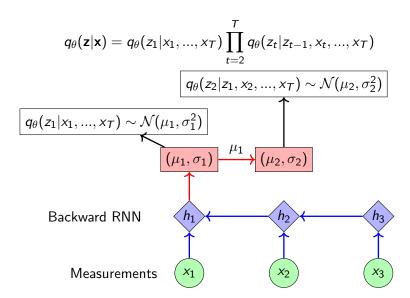
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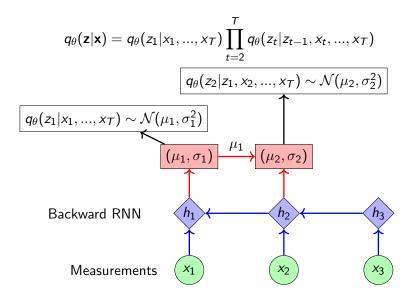




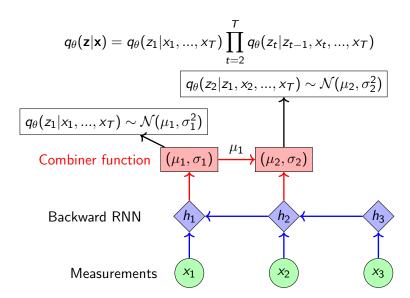




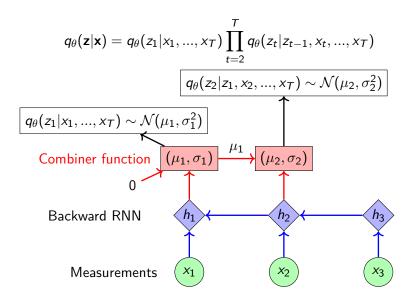




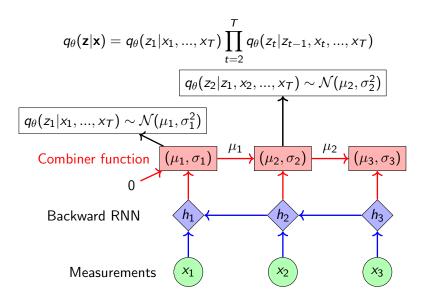




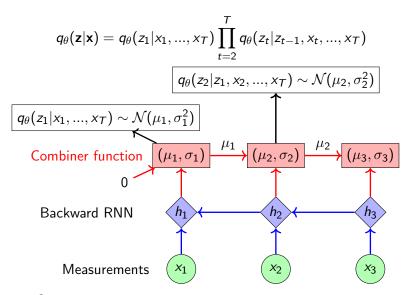












$$ullet$$
 Output: $oldsymbol{\mu}=\mu_1,\mu_2,...,\mu_{\mathcal{T}}$ $oldsymbol{\sigma}=\sigma_1,\sigma_2,...,\sigma_{\mathcal{T}}$



Train the RNN

Maximising the objective function: ELBO

$$\mathcal{L}(\mathsf{x}, \boldsymbol{\mu}, \boldsymbol{\sigma}) = \mathcal{L}(\mathsf{x}, heta)$$



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▶ Maximising the objective function: ELBO

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• Use the noisy gradients to update θ

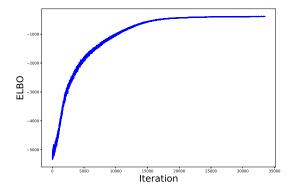


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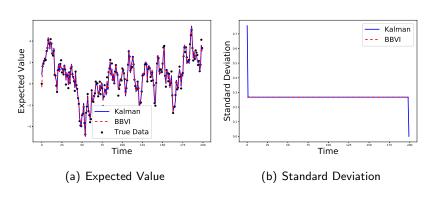
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Results



Conclusions



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- ▶ Our BBVI using a RNN recovers the full posterior probability density function obtained by the Kalman smoother.
- ▶ BBVI using RNN is more flexible than the Kalman smoother, because it can also be used for non-linear SSM with noise that is not Gaussian. All we need to do is to rewrite the ELBO according to the new model.

Thank you for listening!



Any questions?