Probabilistic & Bayesian deep learning

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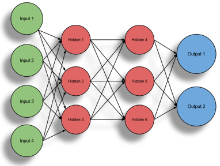
Amazon Research Cambridge, UK

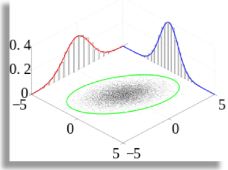
Talk at University of Sheffield, 19 March 2019

In this talk

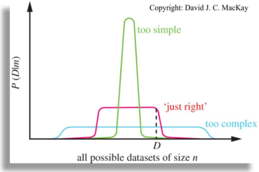
Deep learning



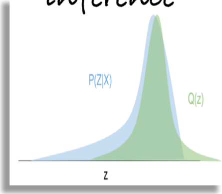
Probabilistic modeling



Bayesian reasoning



Approximate inference



Not in this talk: CRFs, Boltzmann machines, …

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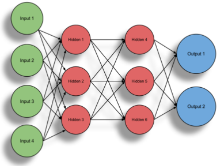

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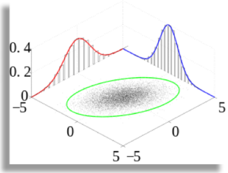

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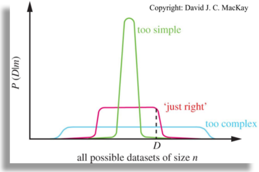

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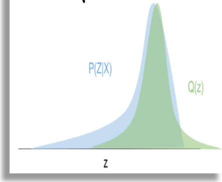

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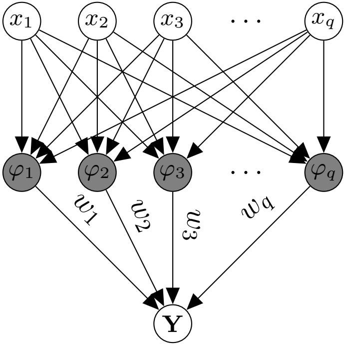
A standard neural network



- Define: $\phi_j = \phi(x_j)$ and $f_j = w_j \phi_j$ (ignore bias for now)
- Once we've defined all w's with back-prop, then f (and the whole network) becomes deterministic.
- What does that imply?

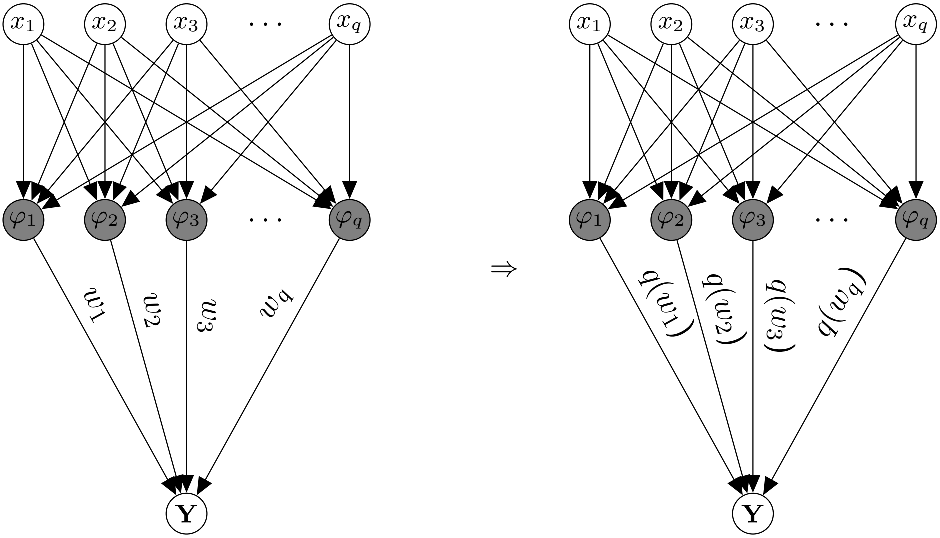
Trained neural network is deterministic. Implications?

- Generalization: Overfitting occurs. Need for ad-hoc invention of regularizers: dropout, early stopping...
- Data generation: A model which generalizes well, should also understand -or even be able to create ("imagine")- variations.
- No predictive uncertainty: Uncertainty needs to be propagated across the model to be reliable.

Need for uncertainty

- Reinforcement learning
- Critical predictive systems
- Active learning
- Semi-automatic systems
- Scarce data scenarios
- ...

BNN with priors on its weights



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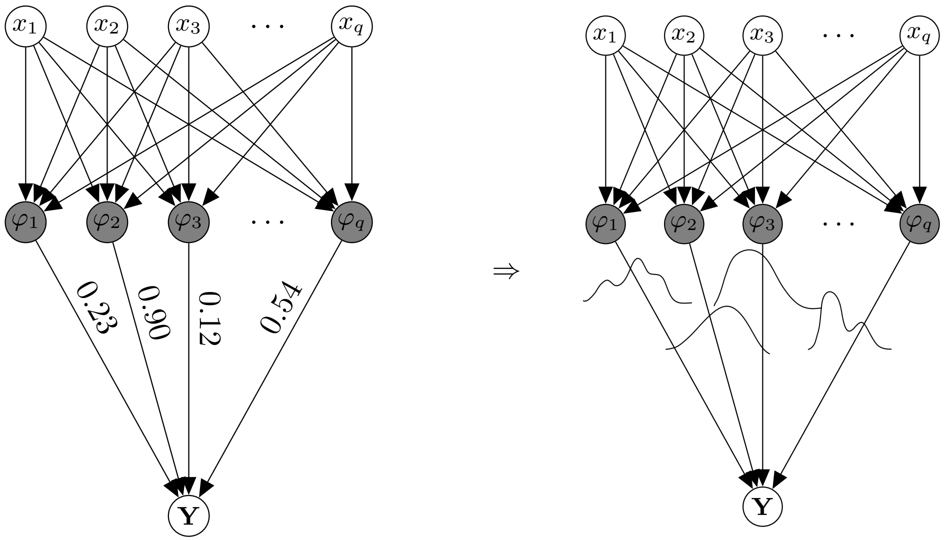

Probabilistic re-formulation

- DNN: $\mathbf{y} = g(\mathbf{W}, \mathbf{x}) = \mathbf{w}_1 \varphi(\mathbf{w}_2 \varphi(\ldots \mathbf{x}))$
- Training minimizing loss:

$$\arg\min_{\mathbf{W}} \underbrace{\frac{1}{2} \sum_{i=1}^{N} (g(\mathbf{W}, x_i) - y_i)^2}_{\text{fit}} + \underbrace{\lambda \sum_i \| \mathbf{w}_i \|}_{\text{regularizer}}$$

- Equivalent probabilistic view for regression, maximizing posterior probability:

$$\arg\max_{\mathbf{W}} \underbrace{\log p(\mathbf{y}|\mathbf{x}, \mathbf{W})}_{\text{fit}} + \underbrace{\log p(\mathbf{W})}_{\text{regularizer}}$$

where $p(\mathbf{y}|\mathbf{x}, \mathbf{W}) \sim \mathcal{N}$ and $p(\mathbf{W}) \sim$ Laplace

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Integrating out weights

- Define: $D = (x, y)$

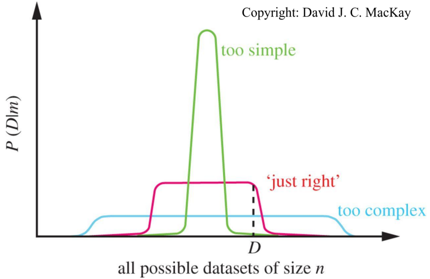
- Remember Bayes' rule:

$$p(w|D) = \frac{p(D|w)p(w)}{p(D) = \int p(D|w)p(w)\mathrm{d}w}$$

- For Bayesian inference, weights need to also be *integrated out*. This gives us a properly defined *posterior* on the parametres.

(Bayesian) Occam's Razor

"A plurality is not to be posited without necessity". *W. of Ockham* "Everything should be made as simple as possible, but not simpler". *A. Einstein*



Evidence is higher for the model that is not "unnecessarily complex" but still "explains" the data D.

Bayesian Inference

Remember: Separation of Model and Inference

Inference

- $p(D)$ (and hence $p(w|D)$) is difficult to compute because of the nonlinear way in which w appears through g.

- Attempt at *variational inference*:

$$\underbrace{\mathsf{KL}\left(q(w;\theta)\,\|\,p(w|D)\right)}_{\text{minimize}} = \log(p(D)) - \underbrace{\mathcal{L}(\theta)}_{\text{maximize}}$$

where

$$\mathcal{L}(\theta) = \underbrace{\mathbb{E}_{q(w;\theta)}[\log p(D,w)]}_{\mathcal{F}} + \mathbb{H}\left[q(w;\theta)\right]$$

- Term in red is still problematic. Solution: MC.

- Such approaches can be formulated as *black-box* inferences.

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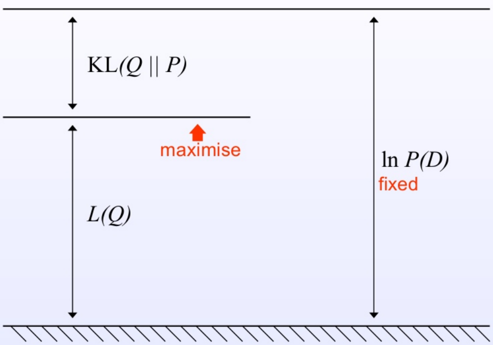
Minimising the KL divergence



Credit: Tushar Tank

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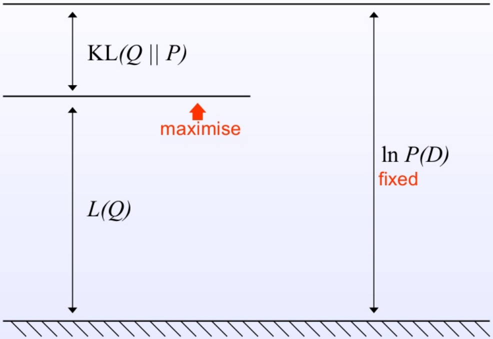

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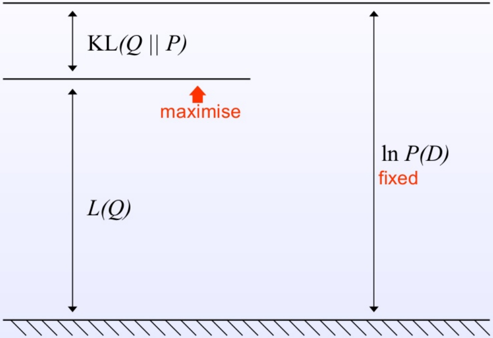

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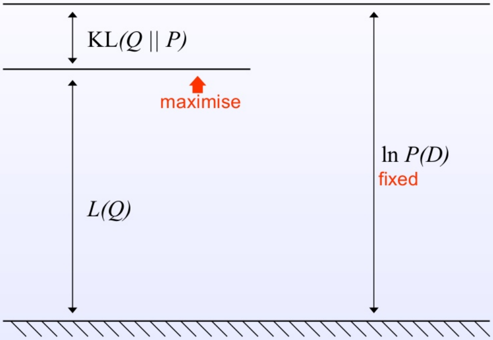

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Inference: "Score function method"

$$
\begin{aligned}
\nabla_\theta \mathcal{F} &= \color{red}{\nabla_\theta \mathbb{E}_{q(w;\theta)}[\log p(D,w)]} \\
&= \mathbb{E}_{q(w;\theta)}\left[p(D,w)\nabla_\theta \log q(w;\theta)\right] \\
&\approx \frac{1}{K}\sum_{i=1}^{K} p(D,w^{(k)})\nabla_\theta \log q(w^{(k)};\theta), \quad w^{(k)} \overset{iid}{\sim} q(w;\theta)
\end{aligned}
$$

(Paisley et al., 2012; Ranganath et al., 2014; Mnih and Gregor, 2014, Ruiz et al. 2016)

Inference: "Reparameterization gradient"

- Reparametrize w as a transformation $\mathcal{T}$ of a simpler variable ϵ: $w = \mathcal{T}(\epsilon; \theta)$
- $q(\epsilon)$ is now independent of θ

$$\begin{aligned}\nabla_\theta \mathcal{F} &= \nabla_\theta \mathbb{E}_{q(w;\theta)}[\log p(D, w)] \\ &= \mathbb{E}_{q(\epsilon)}\left[\nabla_w p(D, w)|_{w=\mathcal{T}(\epsilon;\theta)} \nabla_\theta \mathcal{T}(\epsilon; \theta)\right]\end{aligned}$$

- For example: $w \sim \mathcal{N}(\mu, \sigma) \xrightarrow{\mathcal{T}} w = \mu + \sigma \cdot \epsilon$, $\epsilon \sim \mathcal{N}(0, 1)$
- MC by sampling from $q(\epsilon)$ (thus obtaining samples from w through $\mathcal{T}$)

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Black-box VI

Black-Box Stochastic Variational Inference in Five Lines of Python

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Harvard University

Abstract

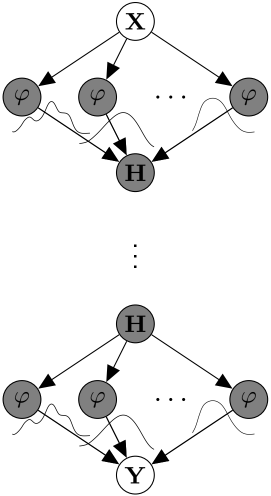
Several large software engineering projects have been undertaken to support black-box inference methods. In contrast, we emphasize how easy it is to construct scalable and easy-to-use automatic inference methods using only automatic differentiation. We present a small function which computes stochastic gradients of the evidence lower bound for any differentiable posterior. As an example, we perform stochastic variational inference in a deep Bayesian neural network.

Black-box VI (github.com/blei-lab/edward)

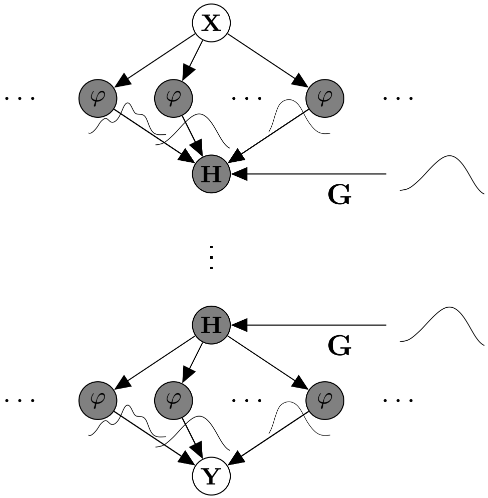
```
# MODEL
W_0 = Normal(loc=tf.zeros([D, 10]), scale=tf.ones([D, 10]))
W_1 = Normal(loc=tf.zeros([10, 10]), scale=tf.ones([10, 10]))
W_2 = Normal(loc=tf.zeros([10, 1]), scale=tf.ones([10, 1]))
b_0 = Normal(loc=tf.zeros(10), scale=tf.ones(10))
b_1 = Normal(loc=tf.zeros(10), scale=tf.ones(10))
b_2 = Normal(loc=tf.zeros(1), scale=tf.ones(1))

X = tf.placeholder(tf.float32, [N, D])
y = Normal(loc=neural_network(X), scale=0.1 * tf.ones(N))

# INFERENCE
qW_0 = Normal(loc=tf.Variable(tf.random_normal([D, 10])),
              scale=tf.nn.softplus(tf.Variable(tf.random_normal([D, 10]))))
```

```
qb_2 = Normal(loc=tf.Variable(tf.random_normal([1])),
              scale=tf.nn.softplus(tf.Variable(tf.random_normal([1]))))

inference = ed.KLqp({W_0: qW_0, b_0: qb_0,
                     W_1: qW_1, b_1: qb_1,
                     W_2: qW_2, b_2: qb_2}, data={X: X_train, y: y_train})
inference.run()
```

Priors on weights *(what we saw before)*



From NN to GP



- NN: $\mathbf{H}_2 = \mathbf{W}_2 \phi(\mathbf{H}_1)$
- GP: ϕ is $\infty-$dimensional so:
  $\mathbf{H}_2 = f_2(\mathbf{H}_1; \theta_2) + \epsilon$
- NN: $p(\mathbf{W})$
- GP: $p(f(\cdot))$
- VAE can be seen as a special case of this

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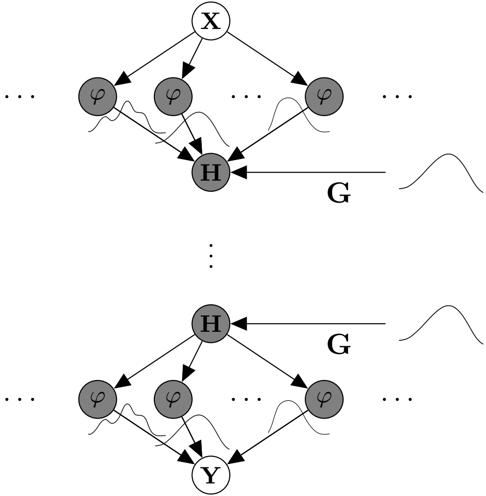

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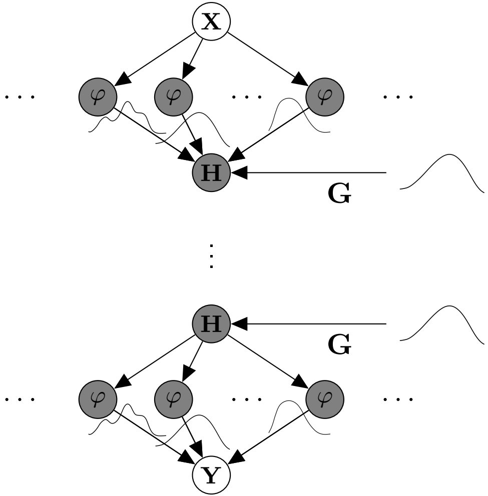

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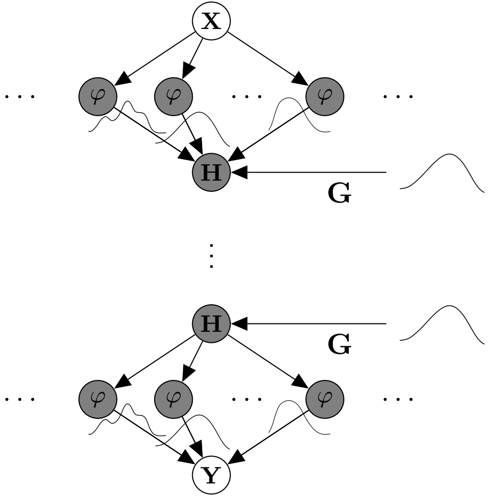


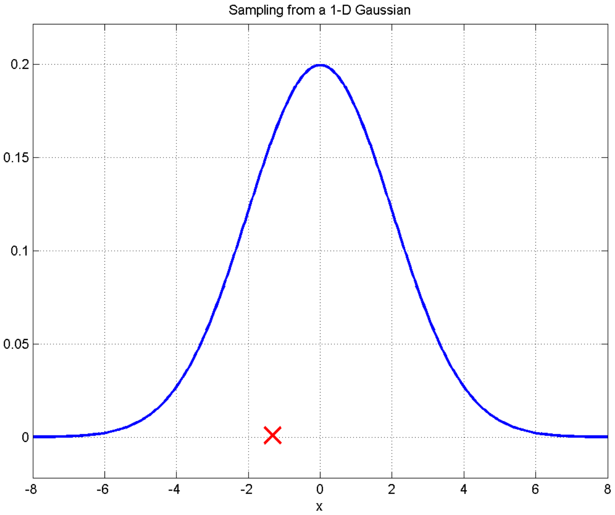
- Real world perfectly described by unobserved *latent* variables: $\hat{\mathbf{H}}$
- But we only observe noisy high-dimensional data: $\mathbf{Y}$
- We try to interpret the world and infer the latents: $\mathbf{H} \approx \hat{\mathbf{H}}$
- Inference:
  $p(\mathbf{H}|\mathbf{Y}) = \frac{p(\mathbf{Y}|\mathbf{H})p(\mathbf{H})}{p(\mathbf{Y})}$

Deep Gaussian processes

- Uncertainty about parameters: Check. Uncertainty about structure?
- Deep GP simultaneously brings in:
  - prior on "weights"
  - input/latent space is kernalized
  - stochasticity in the warping

Introducing Gaussian Processes:

- A Gaussian distribution depends on a mean and a covariance matrix.
- A Gaussian process depends on a mean and a covariance function.



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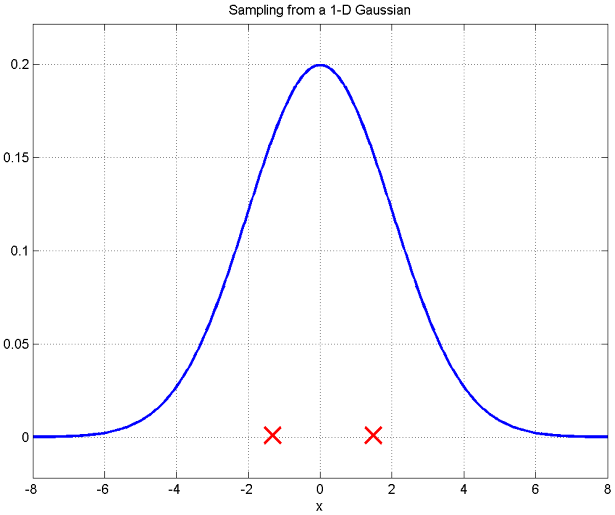
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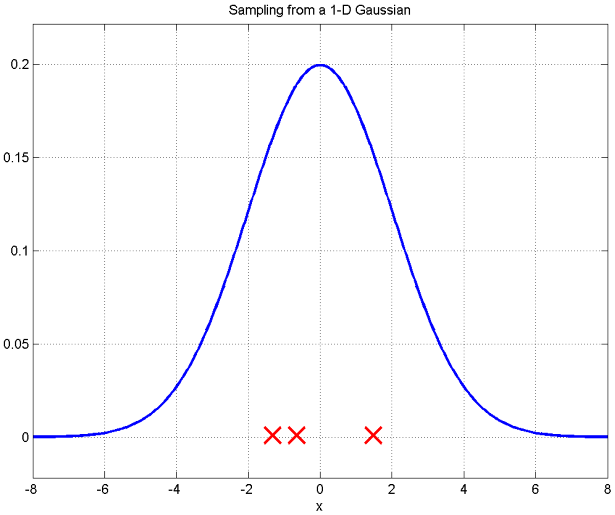
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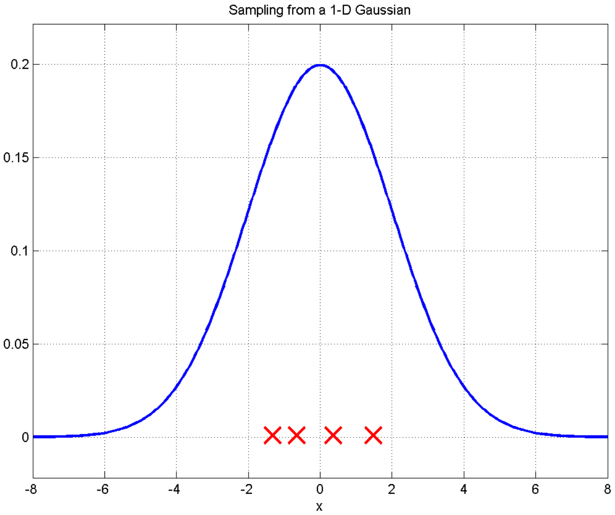
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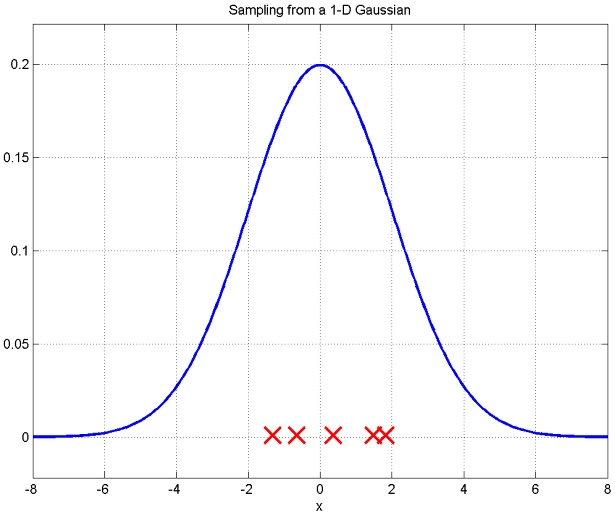
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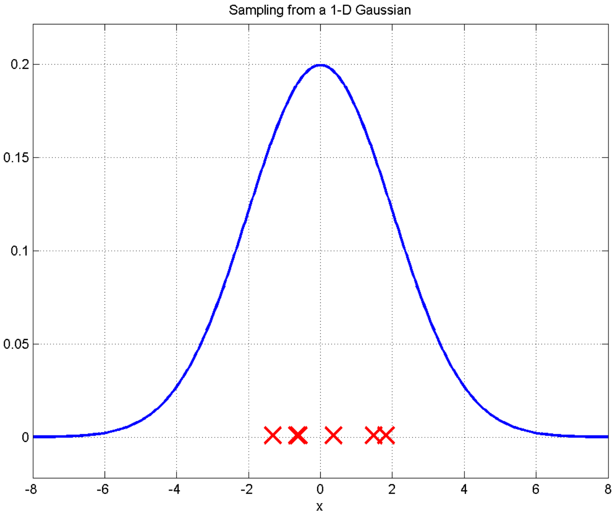

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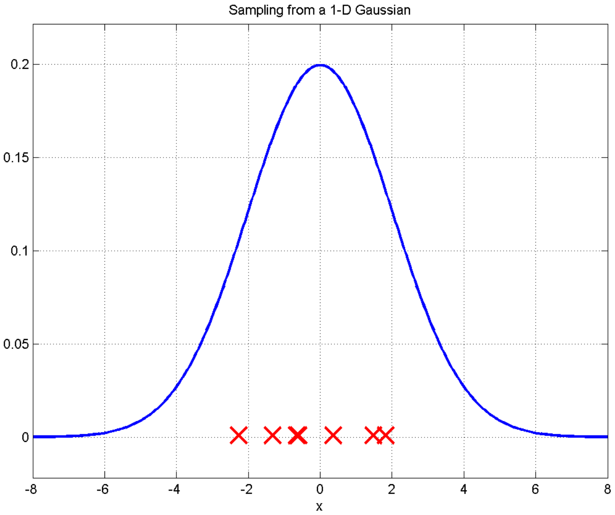
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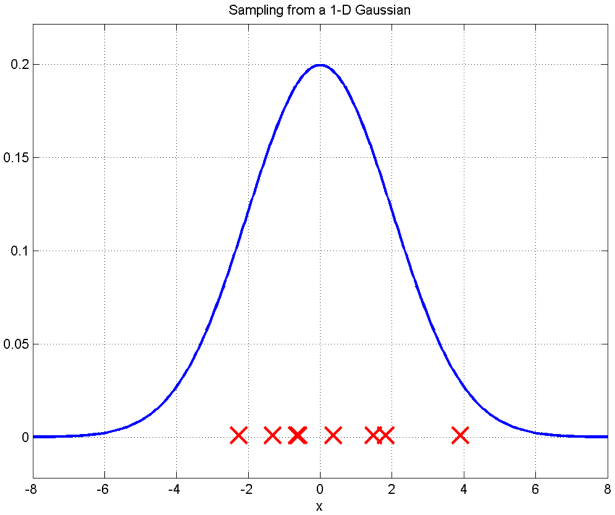
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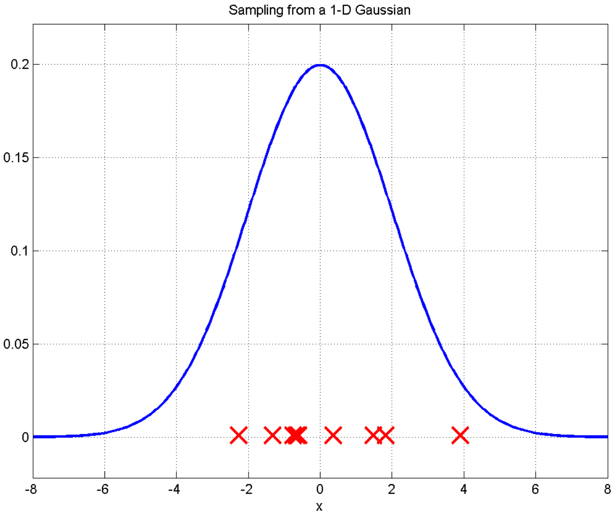
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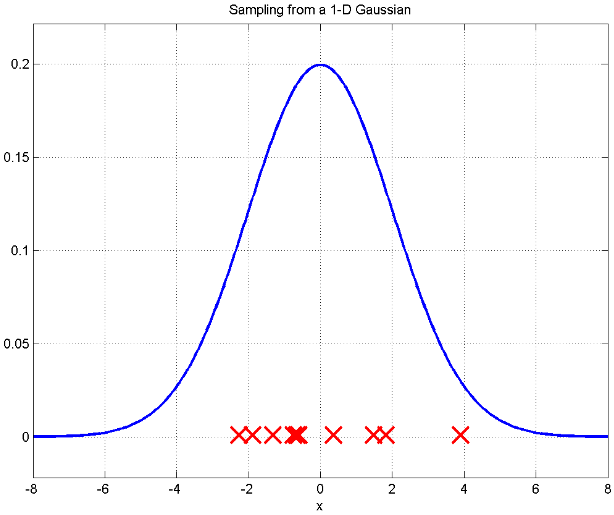

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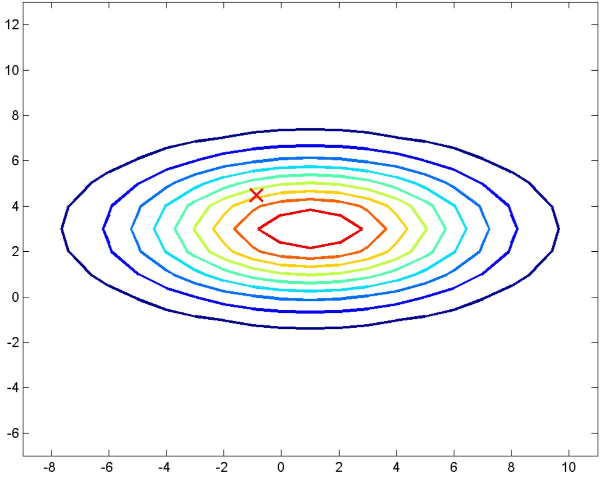
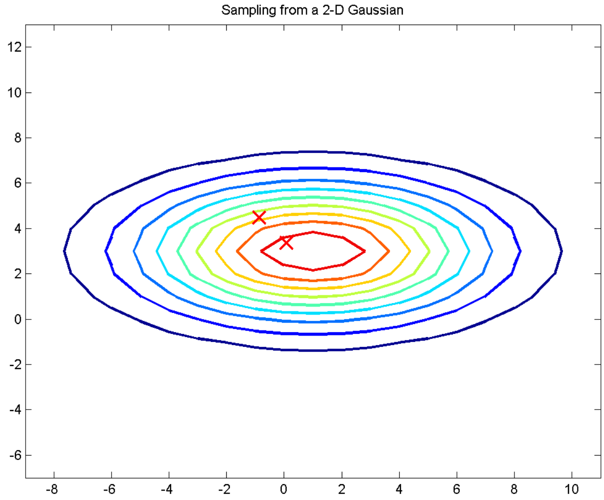
Sampling from a 2-D Gaussian





Sampling from a 2-D Gaussian
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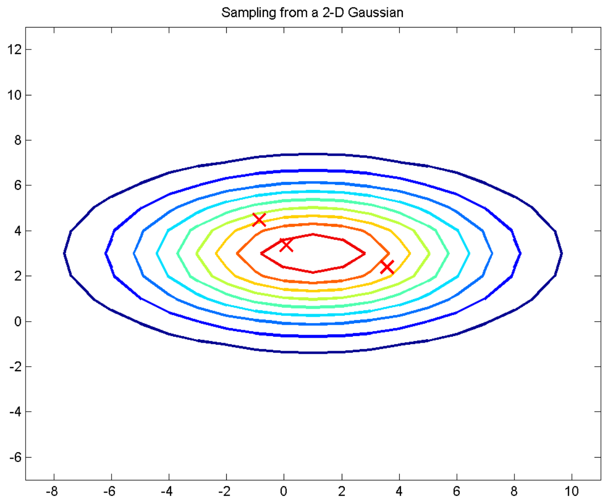

Sampling from a 2-D Gaussian
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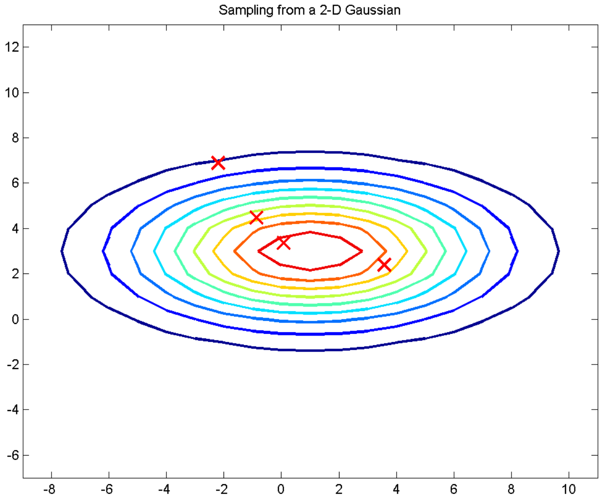

Sampling from a 2-D Gaussian
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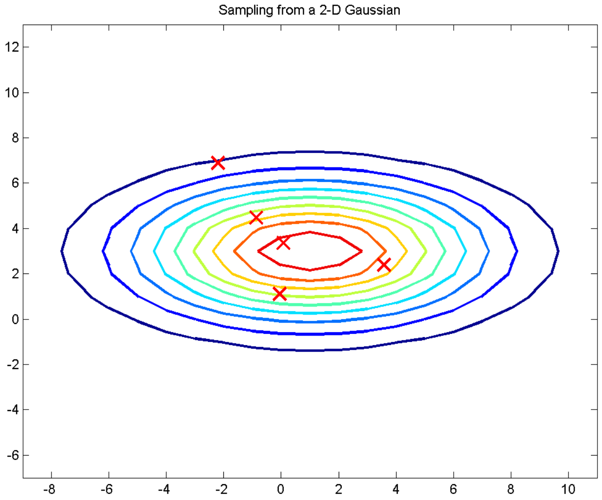
Sampling from a 2-D Gaussian
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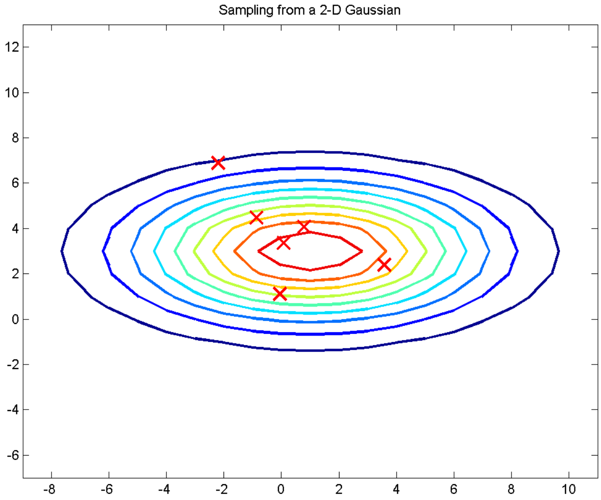

Sampling from a 2-D Gaussian
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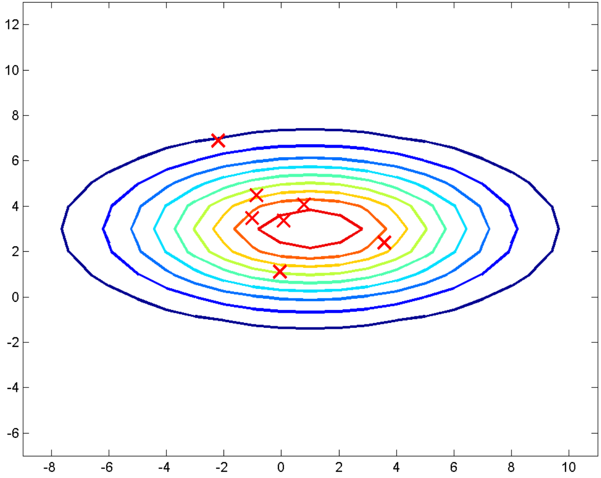
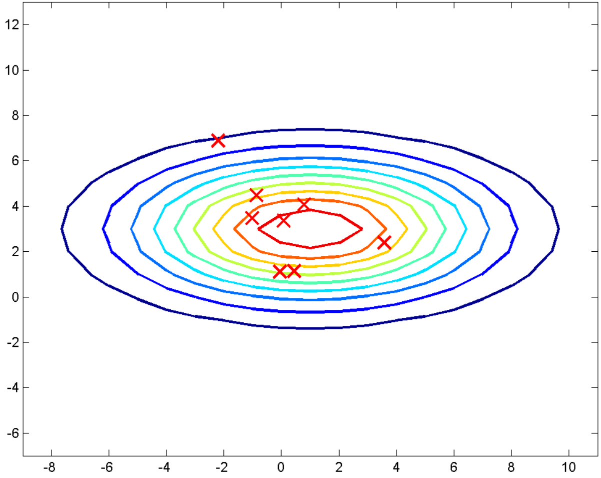
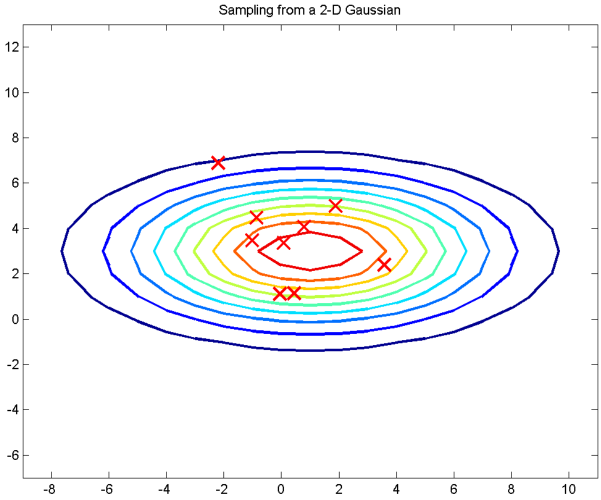
Sampling from a 2-D Gaussian



Sampling from a 2-D Gaussian




Sampling from a 2-D Gaussian
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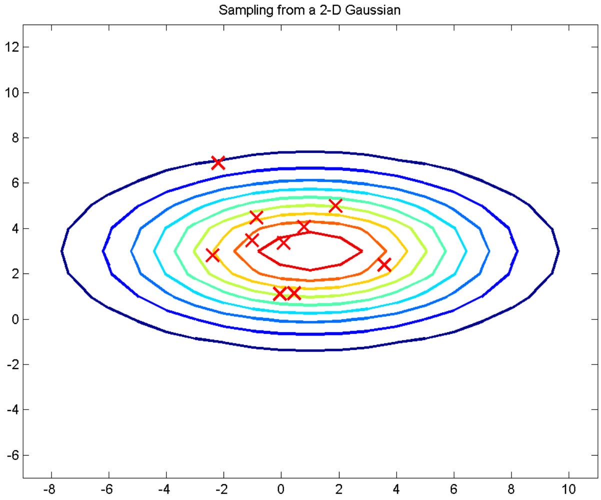
Sampling from a 2-D Gaussian
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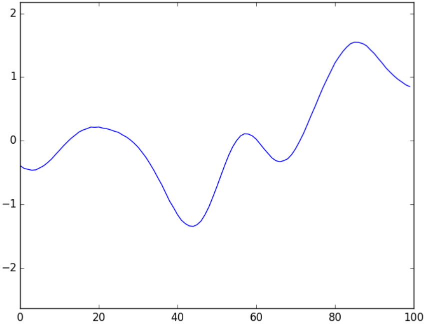
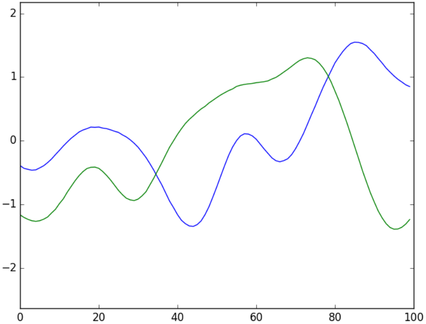
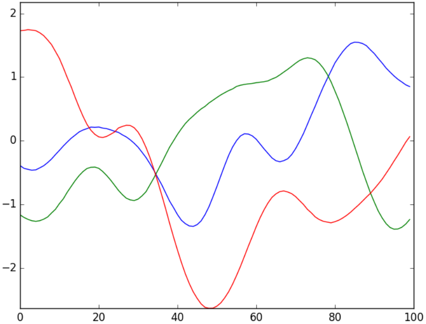
Samples from a 1-D Gaussian



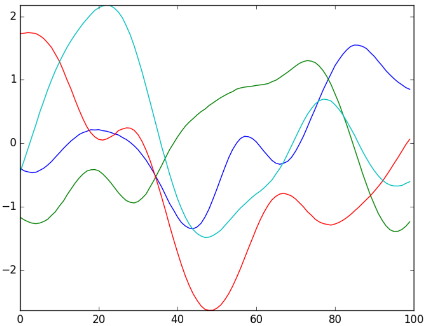
Samples from a 1-D Gaussian



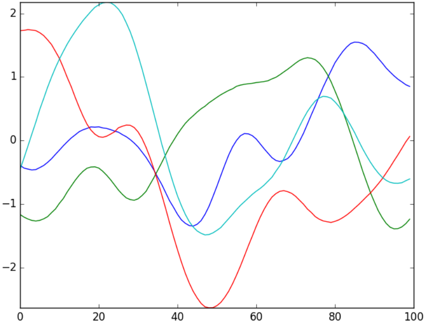
Samples from a 1-D Gaussian

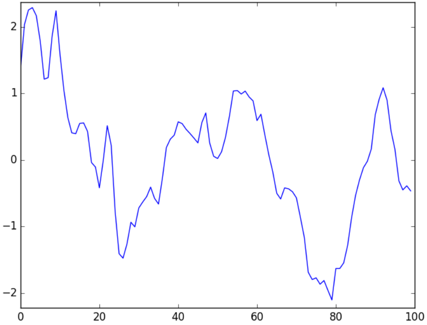


Samples from a 1-D Gaussian

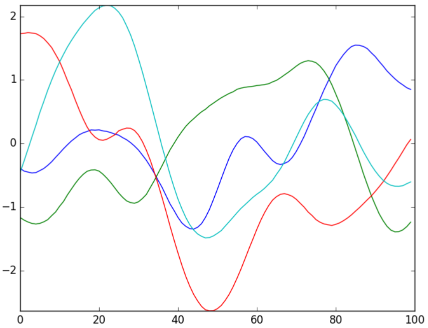


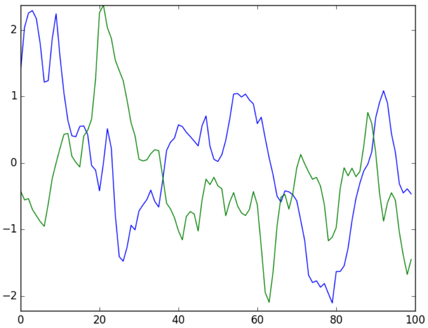
Samples from a 1-D Gaussian



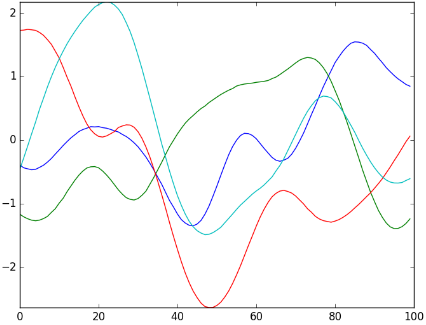


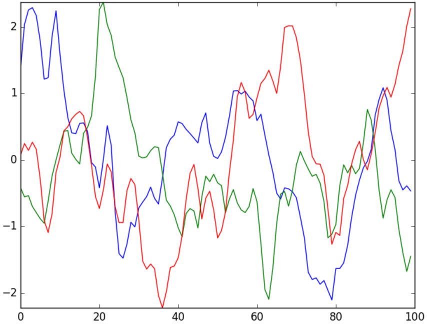
Samples from a 1-D Gaussian



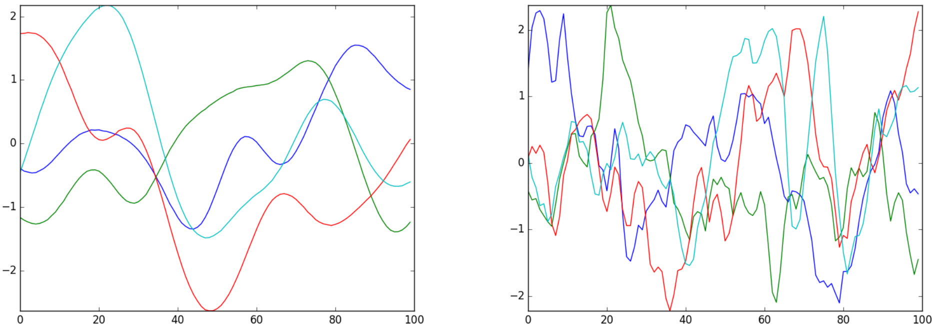


Samples from a 1-D Gaussian





Samples from a 1-D Gaussian



How do GPs solve the overfitting problem (i.e. regularize)?

- Answer: Integrate over the function itself!
- So, we will average out all possible function forms, under a (GP) prior!

Recap:

$$\text{MAP:} \quad \arg\max_{\mathbf{w}} p(\mathbf{y}|\mathbf{w}, \phi(\mathbf{x}))p(\mathbf{w}) \quad \text{e.g. } \mathbf{y} = \phi(\mathbf{x})^\top \mathbf{w} + \boldsymbol{\epsilon}$$

$$\text{Bayesian:} \quad \arg\max_{\boldsymbol{\theta}} \int_{\mathbf{f}} p(\mathbf{y}|\mathbf{f}) \underbrace{p(\mathbf{f}|\mathbf{x}, \boldsymbol{\theta})}_{\text{GP prior}} \quad \text{e.g. } \mathbf{y} = f(\mathbf{x}, \boldsymbol{\theta}) + \boldsymbol{\epsilon}$$

- $\boldsymbol{\theta}$ are *hyper*parameters
- The Bayesian approach (GP) automatically balances the data-fitting with the complexity penalty.

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$$\begin{aligned}
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\text{Bayesian:} \quad & \arg\max_{\boldsymbol{\theta}} \, \int_{\mathbf{f}} p(\mathbf{y}|\mathbf{f}) \underbrace{p(\mathbf{f}|\mathbf{x}, \boldsymbol{\theta})}_{\text{GP prior}} && \text{e.g. } \mathbf{y} = f(\mathbf{x}, \boldsymbol{\theta}) + \boldsymbol{\epsilon}
\end{aligned}$$

- $\boldsymbol{\theta}$ are *hyper*parameters
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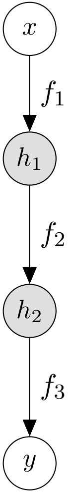
Deep Gaussian processes



- Define a recursive stacked construction

$$f(\mathbf{x}) \rightarrow \text{GP}$$

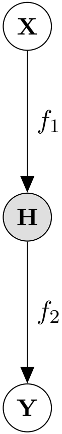
$$f_L(f_{L-1}(f_{L-2} \cdots f_1(\mathbf{x})))) \rightarrow \text{deep GP}$$

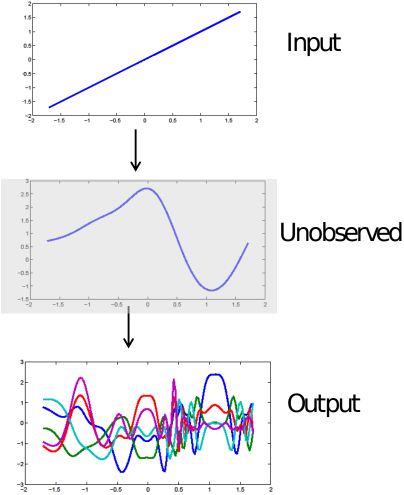
Compare to:

$$\varphi(\mathbf{x})^\top \mathbf{w} \rightarrow \text{NN}$$

$$\varphi(\varphi(\varphi(\mathbf{x})^\top \mathbf{w}_1)^\top \ldots \mathbf{w}_{L-1})^\top \mathbf{w}_L \rightarrow \text{DNN}$$

Two-layered DGP





Inference in DGPs

- It's tricky. An additional difficulty comes from the fact that the kernel couples all points, so $p(y|x)$ is not factorized anymore.

- Indeed, $p(y|x, w) = \int_f p(y|f)p(f|x, w)$ but w appears inside the non-linear kernel function: $p(f|x, w) = N(f|0, k(X, X|w))$

The resulting objective function

By integrating over all unknowns:

- We obtain approximate posteriors $q(h), q(f)$ over them

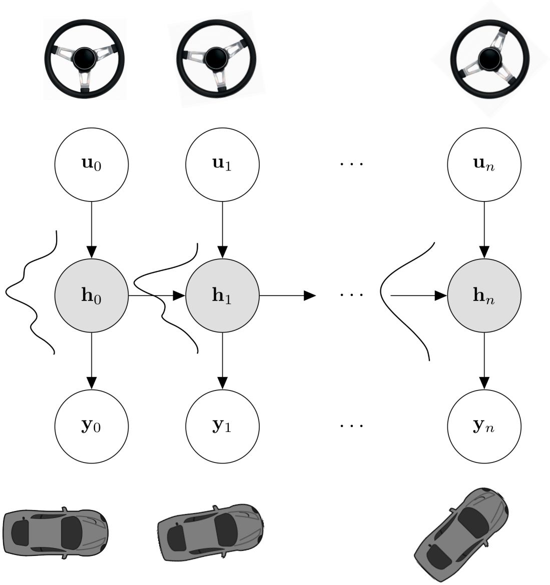
- We end up with a well regularized variational lower bound on the true marginal likelihood:

$$\mathcal{F} = \text{Data Fit} \qquad \underbrace{-\mathsf{KL}\left(q(\mathbf{h}_1) \,\|\, p(\mathbf{h}_1)\right)}_{\text{Regularisation}} + \sum_{l=2}^{L} \underbrace{\mathcal{H}\left(q(\mathbf{h}_l)\right)}_{\text{Regularisation}}$$

- Regularization achieved through uncertainty propagation.

An example where uncertainty propagation matters: Recurrent learning.

Dynamics/memory: Deep Recurrent Gaussian Process



Avatar control

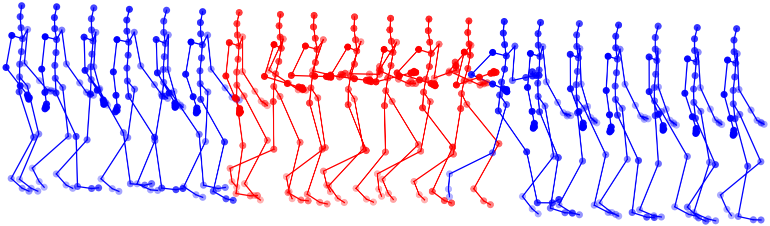


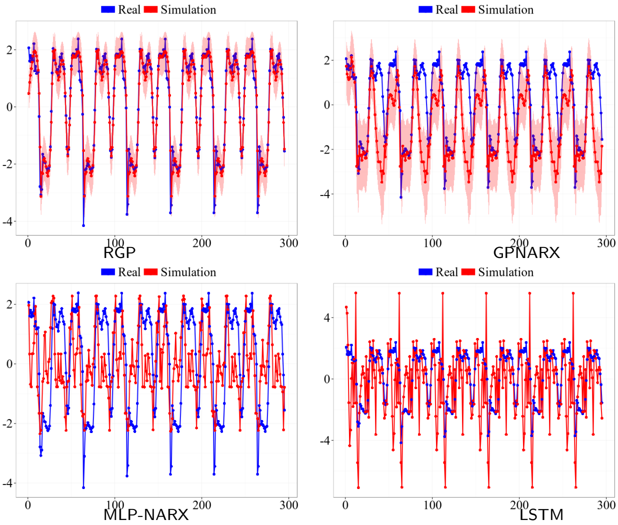
Figure: The generated motion with a step function signal, starting with walking (blue), switching to running (red) and switching back to walking (blue).

Videos:

https://youtu.be/FR-oeGxV6yY *Switching between learned speeds*

https://youtu.be/AT0HMtoPgjc *Interpolating (un)seen speed*

https://youtu.be/FuF-uZ83VMw Constant unseen speed


Real Simulation
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-2
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200
300
RGP
Real Simulation
2
0
-2
-4
0
100
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300
GPNARX
Real Simulation
2
0
-2
-4
0
100
200
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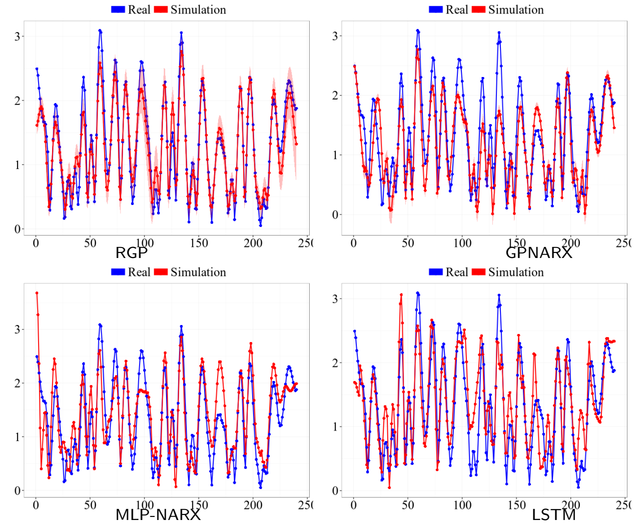
MLP-NARX
Real Simulation
4
0
-4
0
100
200
300
LSTM


Real
Simulation
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RGP
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GPNARX
Real
Simulation
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MLP-NARX
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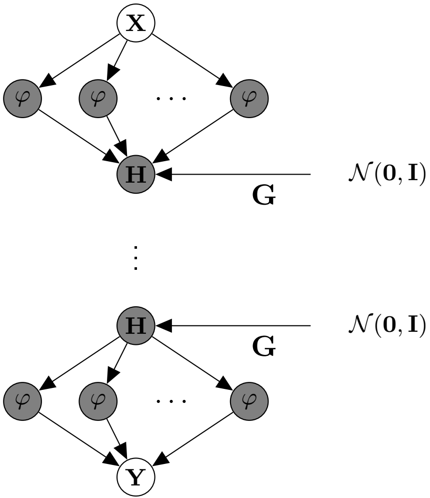
LSTM

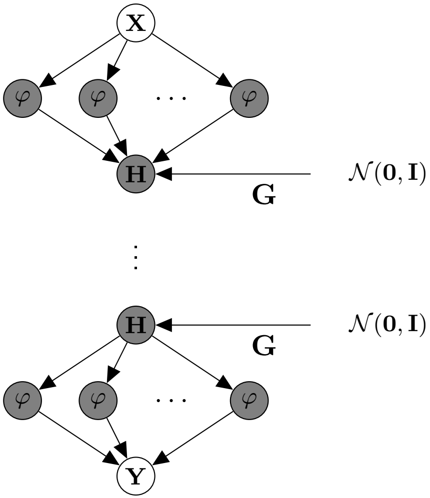
Stochastic warping



Inference:

- Need to infer posteriors on $\mathbf{H}$
- Define $q(\mathbf{H}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- Amortize: $\{\boldsymbol{\mu}, \boldsymbol{\Sigma}\} = MLP(\mathbf{Y}; \boldsymbol{\theta})$

Stochastic warping



Inference:

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- Define $q(\mathbf{H}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- Amortize:
  $\{\boldsymbol{\mu}, \boldsymbol{\Sigma}\} = MLP(\mathbf{Y}; \boldsymbol{\theta})$

Amortized inference

Solution: Reparameterization through recognition model g:

$$
\begin{aligned}
\boldsymbol{\mu}_1^n &= g_1(\mathbf{y}^{(n)}) \\
\boldsymbol{\mu}_l^{(n)} &= g_l(\boldsymbol{\mu}_{l-1}^{(n)}) \\
g_l &= \mathsf{MLP}(\boldsymbol{\theta}_l)
\end{aligned}
$$

g_l deterministic $\Rightarrow \boldsymbol{\mu}_l^{(n)} = g_l(\ldots g_1(\mathbf{y}^{(n)}))$

Dai, Damianou, Gonzalez, Lawrence, ICLR 2016

Bayesian approach recap

- Three ways of introducing uncertainty / noise in a NN:
  - Treat weights w as *distributions* (BNNs)
  - Stochasticity in the warping function ϕ (VAE)
  - Bayesian non-parametrics applied to DNNs (DGP)

Connection between Bayesian and "traditional" approaches

There's another view of Bayesian NNs. Namely that they can be used as a means of explaining / motivating DNN techniques (e.g. Dropout) in a more mathematically grounded way.

- Dropout as variational inference. (Kingma et al. 2015), (Gal and Ghahramani. 2016)
- Low-rank NN weight approximation and Deep Gaussian processes (Hensman and Lawrence 2014, Damianou 2015, Louizos and Welling 2016, Cutajar et al. 2016)
- ...

Summary

- Motivation for probabilistic and Bayesian reasoning
- Three ways of incorporating uncertainty in DNNs
- Inference is more challenging when uncertainty has to be propagated
- Connection between Bayesian and “traditional” NN approaches