Unsupervised Learning with Gaussian Processes

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http://www.carlhenrik.com

Introductions

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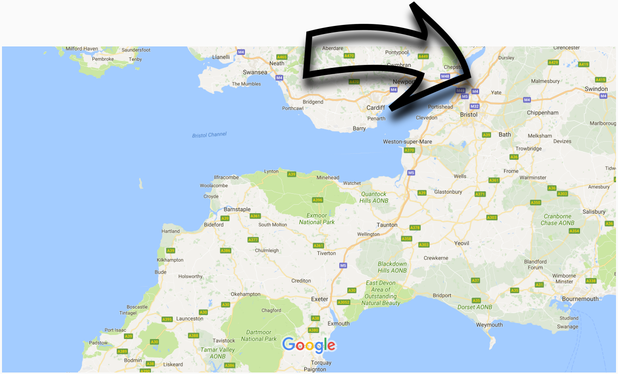
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BLACKTHORN
A DISTINCTIVE CRISP, DRY TASTE
FROM ENGLISH CIDER APPLES
IMPORTED
Fermented Hard Cider
PRODUCT OF IRELAND
500mL / 16.9 fl. oz. 6% ALC./VOL.
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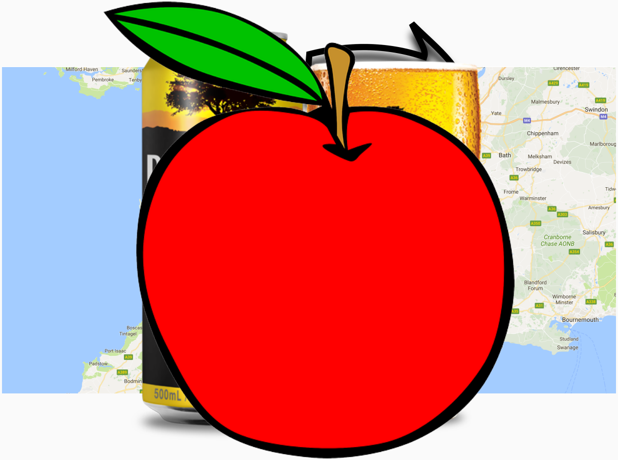
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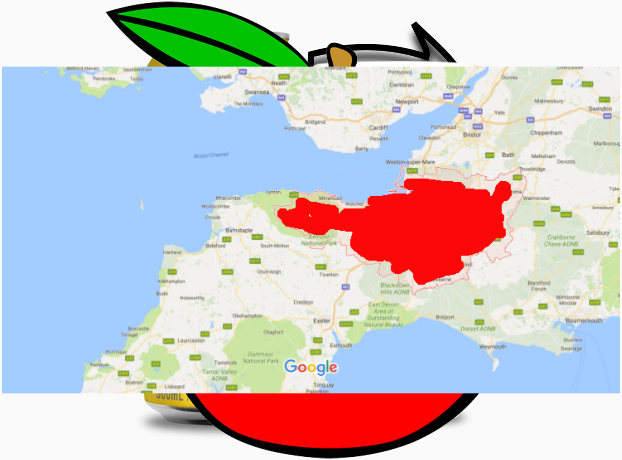
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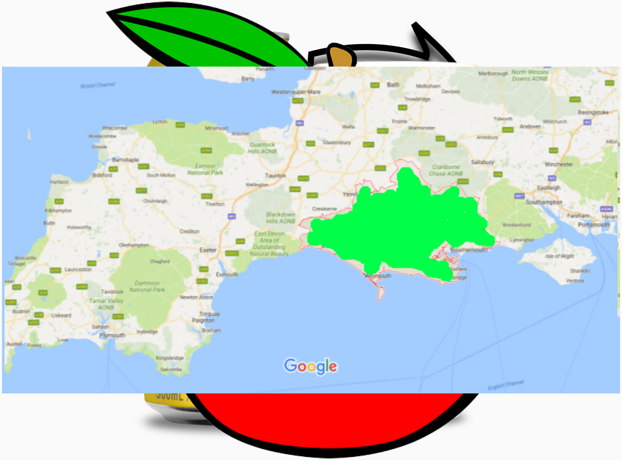
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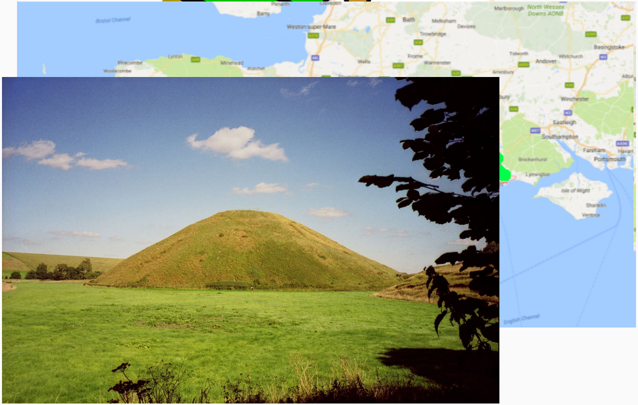
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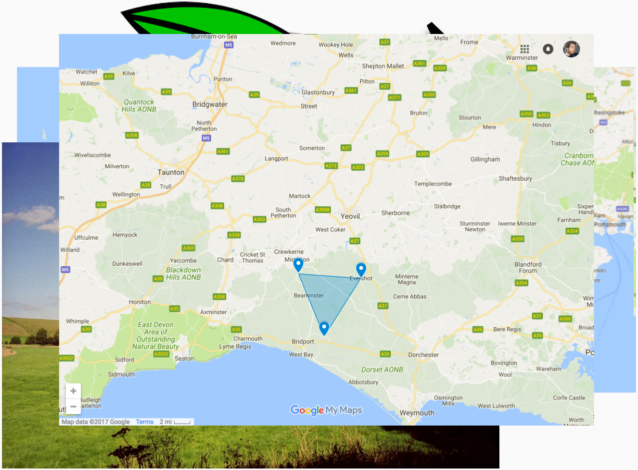
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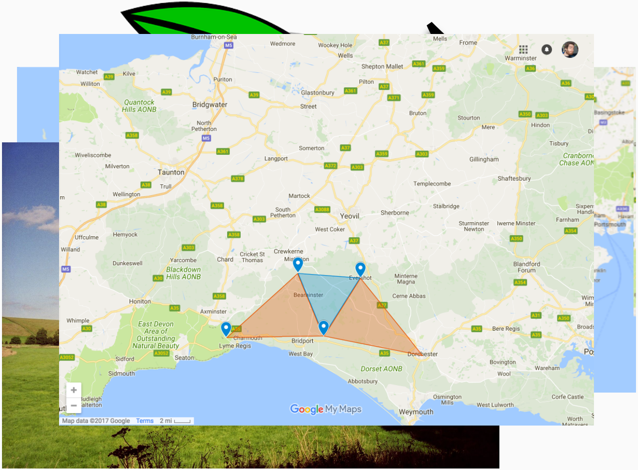
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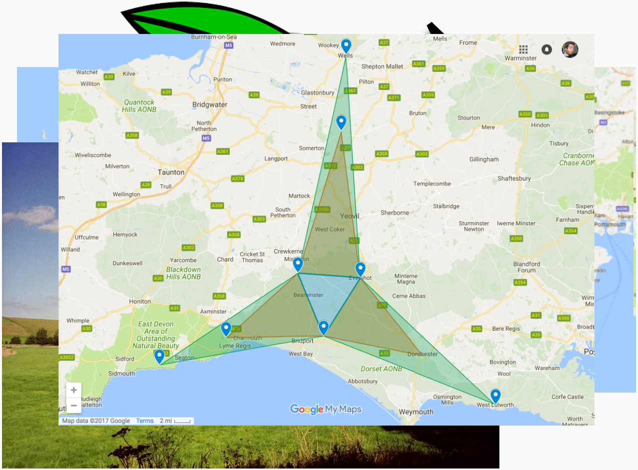
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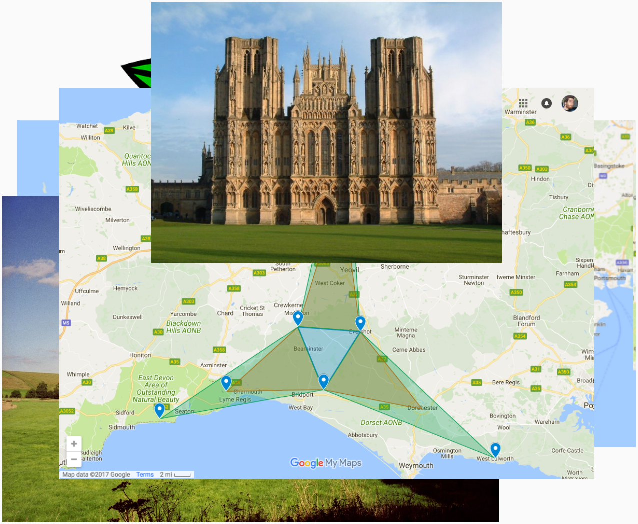
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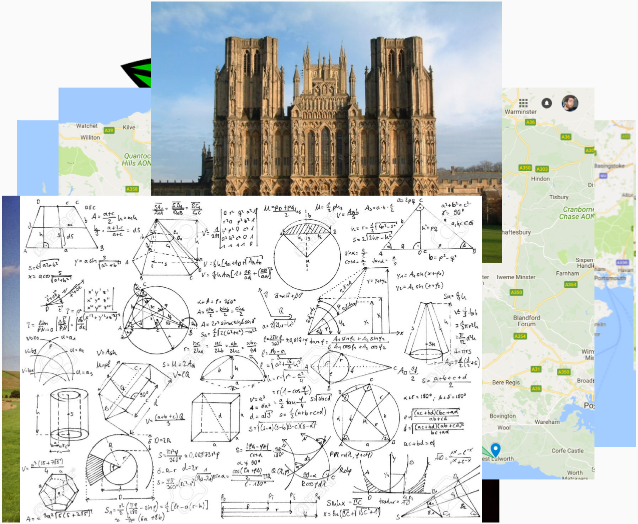
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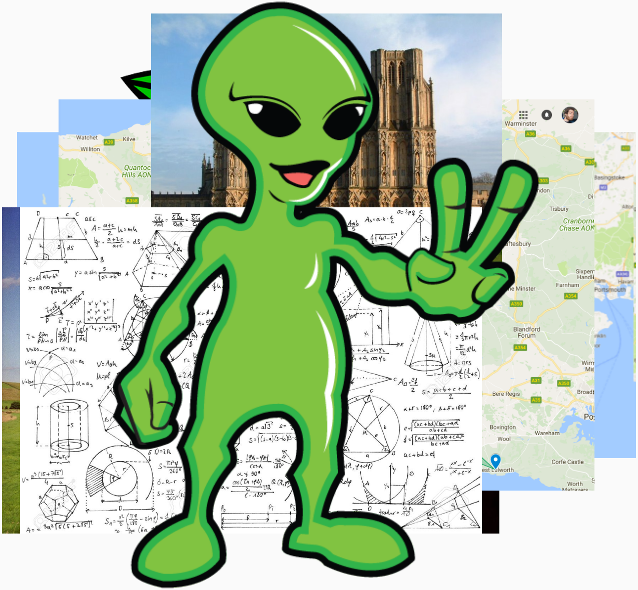
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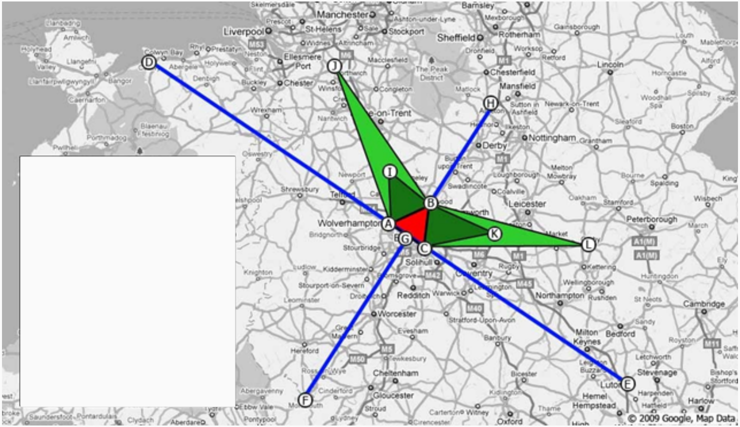
"Brooks has proved, he explains, that there were keen mathematicians here 5,000 years ago, millennia before the Greeks invented geometry: "Such is the mathematical precision, it is inconceivable that this work could have been carried out by the primitive indigenous culture we have always associated with such structures . . . all this suggests a culture existing in these islands in the past quite outside our expectation and experience today." He does not rule out extraterrestrial help." – The Guardian



[1]Bad Science Blog

"We know so little about the ancient Woolworths stores," he explains, "but we do still know their locations. I thought that if we analysed the sites we could learn more about what life was like in 2008 and how these people went about buying cheap kitchen accessories and discount CDs" – Matt Parker interviewed in The Guardian[1]

[1] Bad Science Blog


Lord Nelson
PALE ALE

Napoleon *"You have written this huge book on the system of the world without once mentioning the author of the universe."*

Napoleon *"You have written this huge book on the system of the world without once mentioning the author of the universe."*

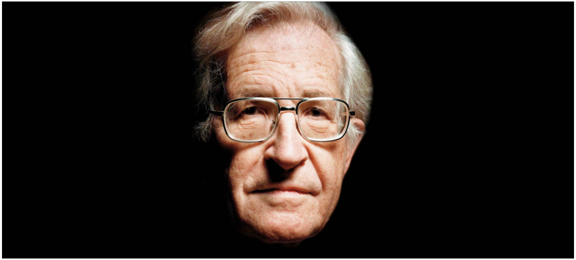
Laplace *"I had no need for that assumption"*

Napoleon *"You have written this huge book on the system of the world without once mentioning the author of the universe."*

Laplace *"I had no need for that assumption"*

Laplace *"Ah, but that is a fine hypothesis. It explains so many things"*

Inductivist Fallacy



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[2]Chomsky, N. A., & Fodor, J. A. (1980). The inductivist fallacy. Language and Learning: The Debate between Jean Piaget and Noam Chomsky, (), .

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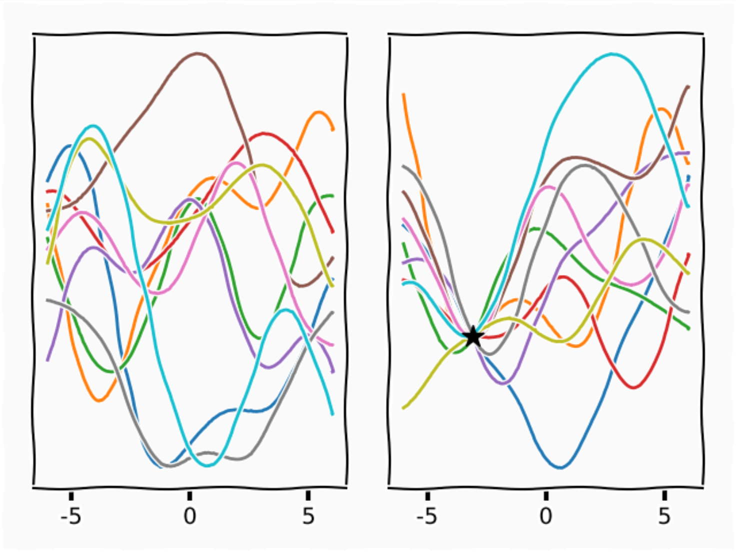
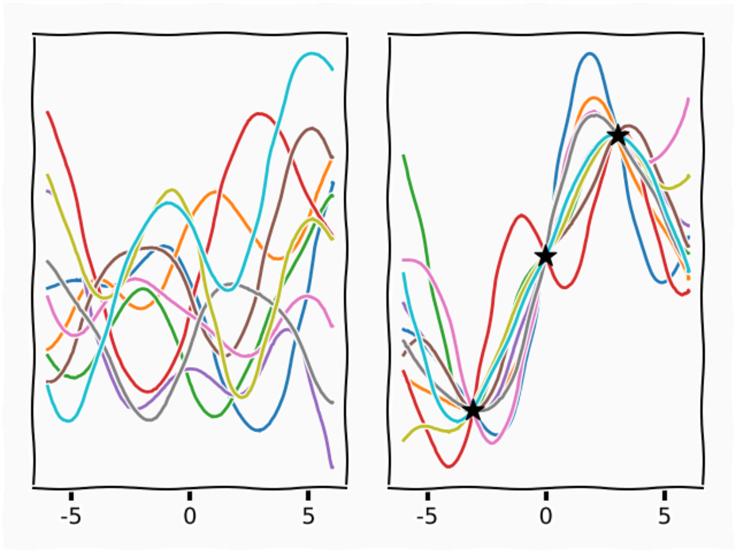
Unsupervised Learning

Gaussian Processes



Gaussian Processes

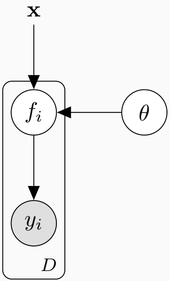


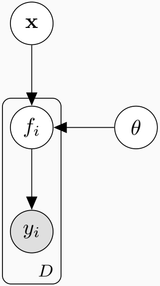
$$p(\theta|y) = p(y|\theta)\frac{p(\theta)}{p(y)}$$

"Scientific modelling is a scientific activity, the aim of which is to make a particular part or feature of the world easier to understand, define, quantify, visualize, or simulate by referencing it to existing and usually commonly accepted knowledge." [3]

[3] Wikipedia

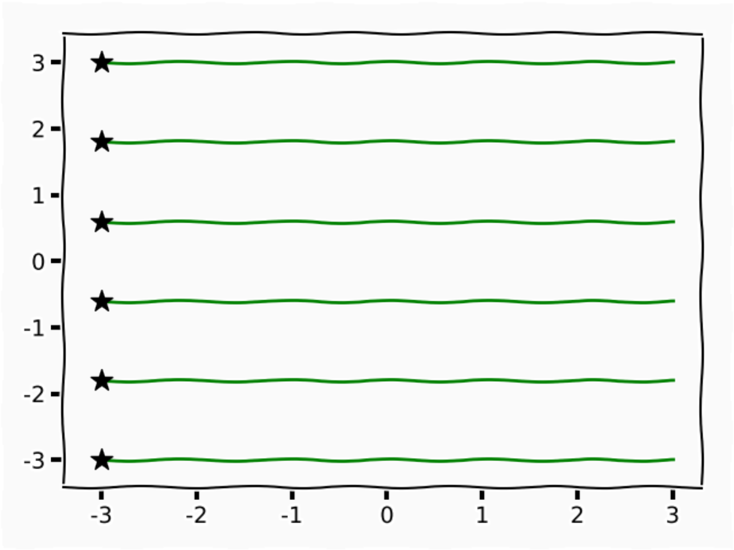
Unsupervised Learning





$p(y|x)$ $p(y)$

Unsupervised Learning



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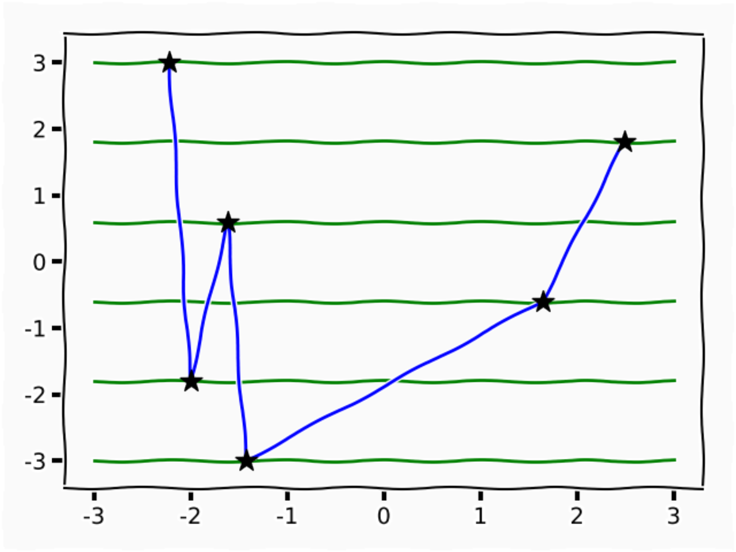

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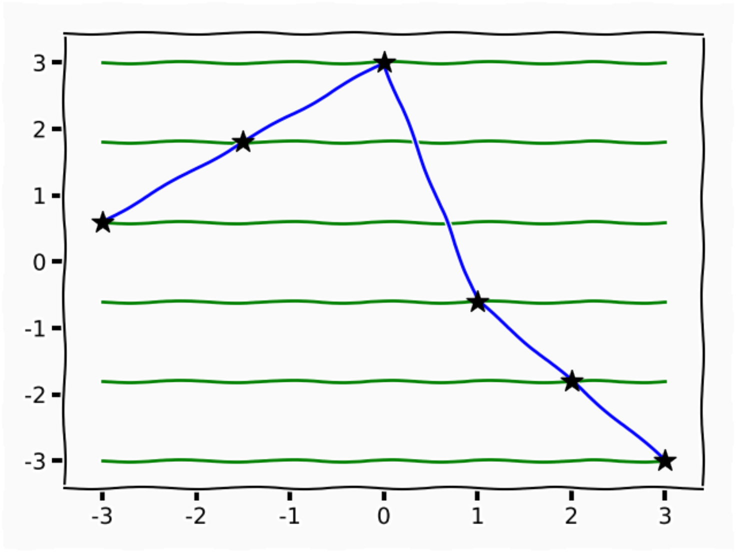

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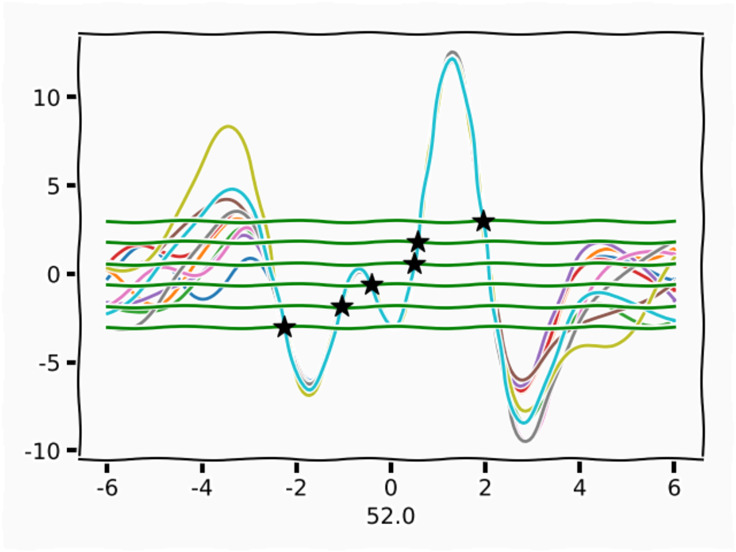

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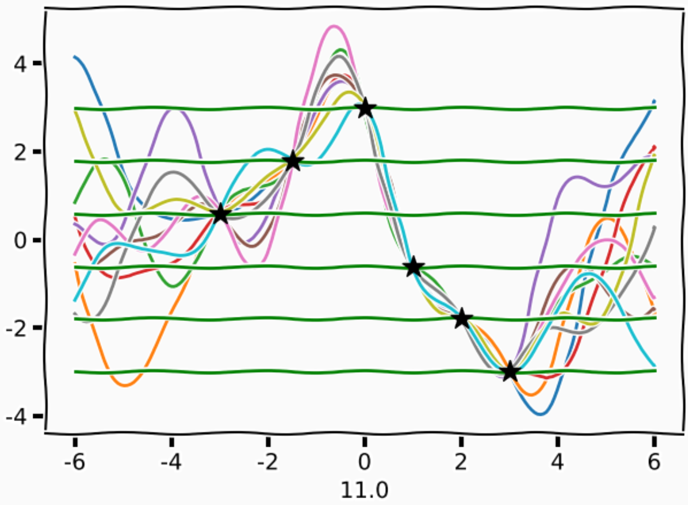

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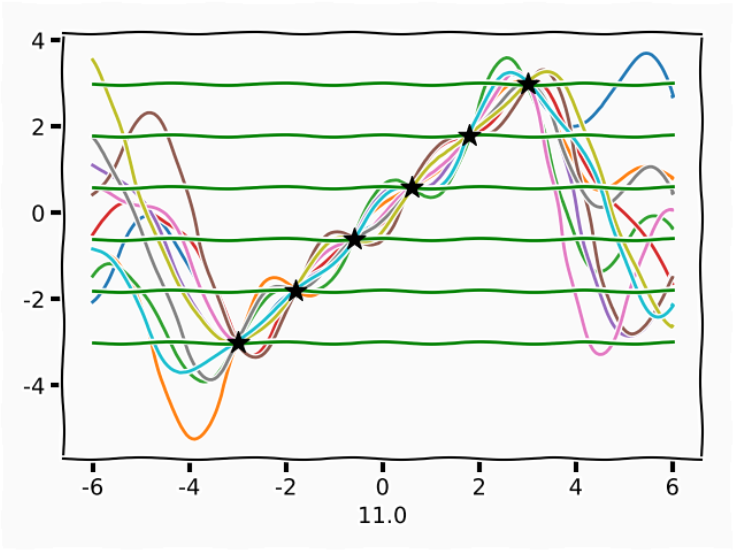

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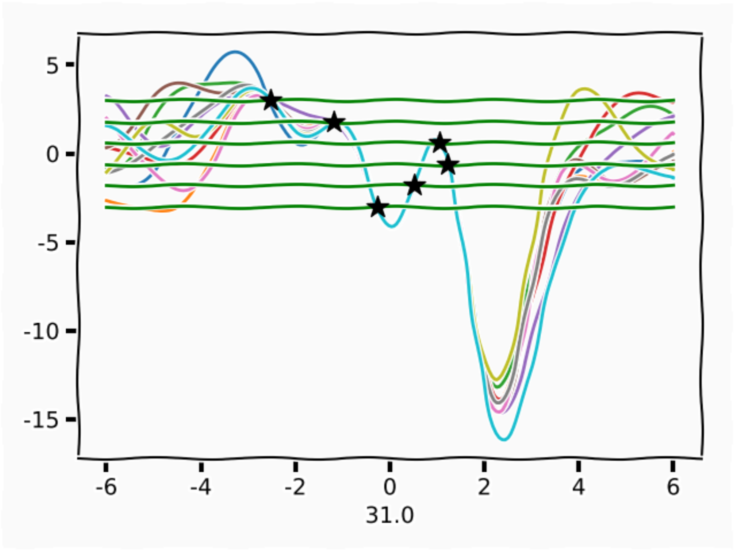

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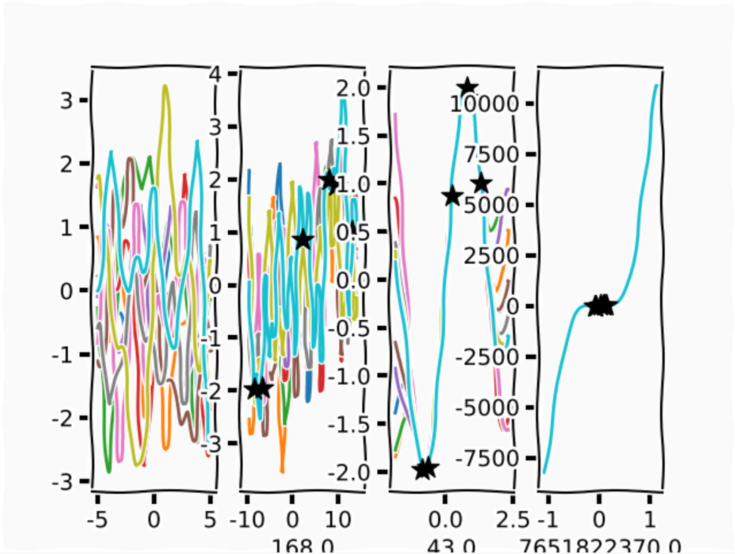


Being Bayesian[4]

[4] By Dieric Bouts (circa 1420-1475) - The Yorck Project: 10.000 Meisterwerke der Malerei, Public Domain, URL

Priors

$$p(y) = \int p(y|f)p(f|x)p(x)\mathrm{d}f\mathrm{d}x$$

$$p(x|y) = p(y|x)\frac{p(x)}{p(y)}$$

1. Priors that makes sense

   p(f) describes our belief/assumptions and defines our notion of complexity in the function

   p(x) expresses our belief/assumptions and defines our notion of complexity in the latent space

2. The priors are *"balanced"*
3. Now lets churn the handle

Relationship between x and data

$$p(y) = \int p(y|f)p(f|x)p(x)\mathrm{d}f\,\mathrm{d}x$$

- GP prior

$$p(f|x) \sim \mathcal{N}(0, K) \propto e^{-\frac{1}{2}(f^{\mathrm{T}}K^{-1}f)}$$

$$K_{ij} = e^{-(x_i - x_j)^{\mathrm{T}}M^{\mathrm{T}}M(x_i - x_j)}$$

Relationship between x and data

$$p(y) = \int p(y|f)p(f|x)p(x)\mathrm{d}f\mathrm{d}x$$

- GP prior

$$p(f|x) \sim \mathcal{N}(0, K) \propto e^{-\frac{1}{2}(f^{\mathrm{T}}K^{-1}f)}$$

$$K_{ij} = e^{-(x_i - x_j)^{\mathrm{T}}M^{\mathrm{T}}M(x_i - x_j)}$$

- Likelihood

$$p(y|f) \sim N(y|f, \beta) \propto e^{-\frac{1}{2\beta}\mathrm{tr}(y-f)^{\mathrm{T}}(y-f)}$$

Relationship between x and data

$$p(y) = \int p(y|f)p(f|x)p(x)\mathrm{d}f\mathrm{d}x$$

- GP prior

$$p(f|x) \sim \mathcal{N}(0, K) \propto e^{-\frac{1}{2}(f^{\mathrm{T}}K^{-1}f)}$$

$$K_{ij} = e^{-(x_i - x_j)^{\mathrm{T}}M^{\mathrm{T}}M(x_i - x_j)}$$

- Likelihood

$$p(y|f) \sim N(y|f, \beta) \propto e^{-\frac{1}{2\beta}\mathrm{tr}(y-f)^{\mathrm{T}}(y-f)}$$

- Analytically intractable (`Non Elementary Integral`) and infinitely differientiable

Laplace Integration

"Nature laughs at the difficulties of integrations"
– Simon Laplace

Unsupervised Learning with GPs

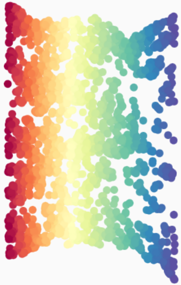
ML/MAP[5]

$$\hat{x} = \text{argmax}_x \int p(y|f)p(f|x)\mathrm{d}f p(x)$$

$$= \text{argmin}_x \frac{1}{2} y^{\mathrm{T}} \mathbf{K}^{-1} y + \frac{1}{2}|\mathbf{K}| - \log\, p(x)$$

[5] Lawrence, N. D. (2005). Probabilistic non-linear principal component analysis with Gaussian process latent variable models.

Dimensionality Reduction



$$y \in \mathbb{R}^d \quad x \in \mathbb{R}^q \quad d > q$$

GP-LVM

- Li, W., Viola, F., Starck, J., Brostow, G. J., & Campbell, N. D. (2016). Roto++: accelerating professional rotoscoping using shape manifolds. (In proceeding of ACM SIGGRAPH'16)
- Grochow, K., Martin, S. L., Hertzmann, A., & Popovi\'c, Zoran (2004). Style-based inverse kinematics. SIGGRAPH '04: SIGGRAPH 2004
- Urtasun, R., Fleet, D. J., & Fua, P. (2006). 3D people tracking with Gaussian process dynamical models. Computer Vision and Pattern Recognition, 2006

Bayesian GP-LVM[7]

- Challenges with ML estimation
  - How to initialise x?
  - What is the dimensionality q?
- *Our assumption on the latent space does not reach the data*

[6] Titsias, M. (2009). Variational learning of inducing variables in sparse Gaussian processes.
[7] Titsias, M., & Lawrence, N. D. (2010). Bayesian Gaussian Process Latent Variable Model

Bayesian GP-LVM[7]

- Challenges with ML estimation
  - How to initialise x?
  - What is the dimensionality q?
- *Our assumption on the latent space does not reach the data*
- Approximate integration![6]

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[7] Titsias, M., & Lawrence, N. D. (2010). Bayesian Gaussian Process Latent Variable Model

Variational Bayes

$$p(\mathbf{Y})$$

Variational Bayes

$$\log p(\mathbf{Y})$$

Variational Bayes

$$\log p(\mathbf{Y}) = \log \int p(\mathbf{Y}, \mathbf{X}) \mathrm{d}\mathbf{X}$$

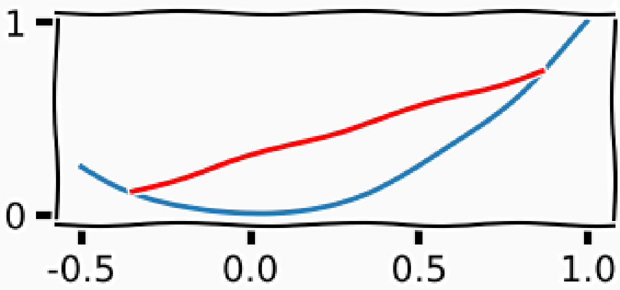
Variational Bayes

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

Variational Bayes

$$\begin{aligned}\log\, p(\mathbf{Y}) &= \log \int p(\mathbf{Y},\mathbf{X})\mathrm{d}\mathbf{X} = \log \int p(\mathbf{X}|\mathbf{Y})p(\mathbf{Y})\mathrm{d}\mathbf{X} \\ &= \log \int \frac{q(\mathbf{X})}{q(\mathbf{X})} p(\mathbf{X}|\mathbf{Y})p(\mathbf{Y})\mathrm{d}\mathbf{X}\end{aligned}$$

Jensen Inequality



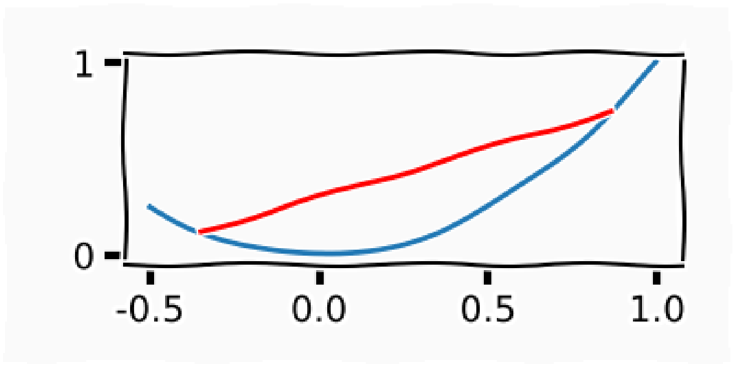
Convex Function

$$\lambda f(x_0) + (1-\lambda) f(x_1) \geq f(\lambda x_0 + (1-\lambda) x_1)$$

$$x \in [x_{min}, x_{max}]$$

$$\lambda \in [0, 1]]$$

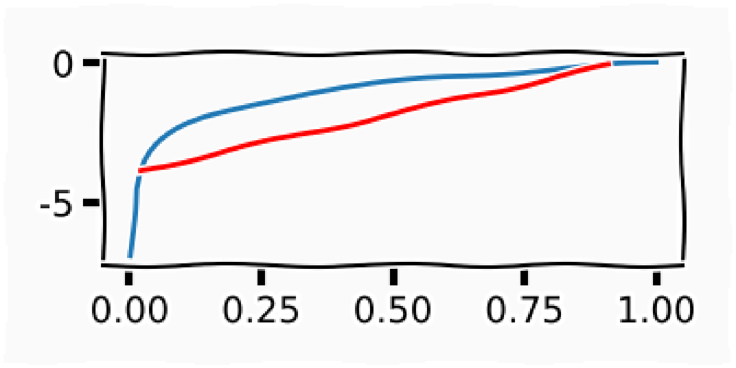
Jensen Inequality



$$\mathbb{E}[f(x)] \geq f(\mathbb{E}[x])$$

$$\int f(x)p(x)\mathrm{d}x \geq f\left(\int xp(x)\mathrm{d}x\right)$$

Jensen Inequality in Variational Bayes



$$\int \log(x)p(x)\mathrm{d}x \leq \log\left(\int xp(x)\mathrm{d}x\right)$$

moving the log inside the the integral is a lower-bound on the integral

Variational Bayes cont.

$$\log p(\mathbf{Y}) = \log \int \frac{q(\mathbf{X})}{q(\mathbf{X})} p(\mathbf{X}|\mathbf{Y}) p(\mathbf{Y}) \mathrm{d}\mathbf{X} =$$

Variational Bayes cont.

$$\begin{aligned}\log p(\mathbf{Y}) &= \log \int \frac{q(\mathbf{X})}{q(\mathbf{X})} p(\mathbf{X}|\mathbf{Y}) p(\mathbf{Y}) \mathrm{d}\mathbf{X} = \\ &\geq \int q(\mathbf{X}) \log \frac{p(\mathbf{X}|\mathbf{Y}) p(\mathbf{Y})}{q(\mathbf{X})} \mathrm{d}\mathbf{X}\end{aligned}$$

Variational Bayes cont.

$$
\begin{aligned}
\log p(\mathbf{Y}) &= \log \int \frac{q(\mathbf{X})}{q(\mathbf{X})} p(\mathbf{X}|\mathbf{Y}) p(\mathbf{Y}) \mathrm{d}\mathbf{X} = \\
&\geq \int q(\mathbf{X}) \log \frac{p(\mathbf{X}|\mathbf{Y}) p(\mathbf{Y})}{q(\mathbf{X})} \mathrm{d}\mathbf{X} \\
&= \int q(\mathbf{X}) \log \frac{p(\mathbf{X}|\mathbf{Y})}{q(\mathbf{X})} \mathrm{d}\mathbf{X} + \int q(\mathbf{X}) \mathrm{d}\mathbf{X} \log\, p(\mathbf{Y})
\end{aligned}
$$

Variational Bayes cont.

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

Variational Bayes cont.

$$
\begin{aligned}
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&= -\mathrm{KL}\left(q(\mathbf{X}) || p(\mathbf{X}|\mathbf{Y})\right) + \log\, p(\mathbf{Y})
\end{aligned}
$$

- if $q(\mathbf{X})$ is the true posterior we have an equality, therefore match the distributions

Variational Bayes cont.

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

- if $q(\mathbf{X})$ is the true posterior we have an equality, therefore match the distributions
- i.e. $\mathrm{argmin}_q \; \mathrm{KL}\left(q(\mathbf{X}) || p(\mathbf{X}|\mathbf{Y})\right)$

  $\Rightarrow$ variational distributions are approximations to intractable posteriors

ELBO

$$\mathrm{KL}(q(\mathbf{X})||p(\mathbf{X}|\mathbf{Y}))$$

ELBO

$$\mathrm{KL}(q(\mathbf{X})||p(\mathbf{X}|\mathbf{Y})) = \int q(\mathbf{X}) log \frac{q(\mathbf{X})}{p(\mathbf{X}|\mathbf{Y})} \mathrm{d}\mathbf{X}$$

ELBO

$$
\begin{aligned}
\mathrm{KL}(q(\mathsf{X})||p(\mathsf{X}|\mathsf{Y})) &= \int q(\mathsf{X}) log \frac{q(\mathsf{X})}{p(\mathsf{X}|\mathsf{Y})} \mathrm{d}\mathsf{X} \\
&= \int q(\mathsf{X}) log \frac{q(\mathsf{X})}{p(\mathsf{X},\mathsf{Y})} \mathrm{d}\mathsf{X} + log\ \ p(\mathsf{Y})
\end{aligned}
$$

ELBO

$$
\begin{aligned}
\mathrm{KL}(q(\mathbf{X})||p(\mathbf{X}|\mathbf{Y})) &= \int q(\mathbf{X}) log \frac{q(\mathbf{X})}{p(\mathbf{X}|\mathbf{Y})} \mathrm{d}\mathbf{X} \\
&= \int q(\mathbf{X}) log \frac{q(\mathbf{X})}{p(\mathbf{X},\mathbf{Y})} \mathrm{d}\mathbf{X} + log\ p(\mathbf{Y}) \\
&= H(q(\mathbf{X})) - \mathbb{E}_{q(\mathbf{X})}\left[log\ p(\mathbf{X},\mathbf{Y})\right] + log\ p(\mathbf{Y})
\end{aligned}
$$

ELBO

$$log\ \ p(\mathbf{Y}) = \mathrm{KL}(q(\mathbf{X})||p(\mathbf{X}|\mathbf{Y})) + \underbrace{\mathbb{E}_{q(\mathbf{X})}\left[log\ \ p(\mathbf{X},\mathbf{Y})\right] - H(q(\mathbf{X}))}_{\mathrm{ELBO}}$$

ELBO

$$log\ p(\mathbf{Y}) = \mathrm{KL}(q(\mathbf{X})||p(\mathbf{X}|\mathbf{Y})) + \underbrace{\mathbb{E}_{q(\mathbf{X})}\left[log\ p(\mathbf{X},\mathbf{Y})\right] - H(q(\mathbf{X}))}_{\mathrm{ELBO}}$$

$$\geq \mathbb{E}_{q(\mathbf{X})}\left[log\ p(\mathbf{X},\mathbf{Y})\right] - H(q(\mathbf{X})) = \mathcal{L}(q(\mathbf{X}))$$

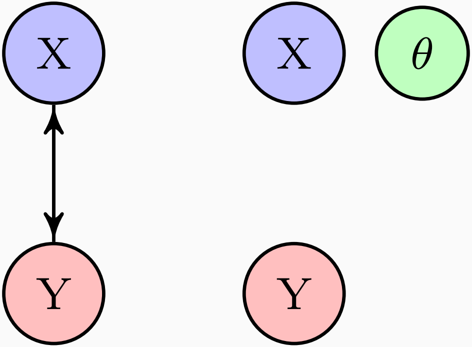
ELBO

$$log\ p(\mathbf{Y}) = \mathrm{KL}(q(\mathbf{X})||p(\mathbf{X}|\mathbf{Y})) + \underbrace{\mathbb{E}_{q(\mathbf{X})}\left[log\ p(\mathbf{X},\mathbf{Y})\right] - H(q(\mathbf{X}))}_{\mathrm{ELBO}}$$

$$\geq \mathbb{E}_{q(\mathbf{X})}\left[log\ p(\mathbf{X},\mathbf{Y})\right] - H(q(\mathbf{X})) = \mathcal{L}(q(\mathbf{X}))$$

- if we maximise the ELBO we,
    - find an approximate posterior
    - get an approximation to the marginal likelihood
- *maximising* $p(\mathbf{Y})$ is learning
- finding $p(\mathbf{X}|\mathbf{Y}) \approx q(\mathbf{X})$ is prediction

ELBO



Why is this useful?

Why is this a sensible thing to do?

- If we can't formulate the joint distribution there isn't much we can do

– Ryan Adams[8]

[8] `Talking Machines Season 2, Episode 5`

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Why is this a sensible thing to do?

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- Taking the expectation of a log is usually easier than the expectation

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Why is this useful?

Why is this a sensible thing to do?

- If we can't formulate the joint distribution there isn't much we can do
- Taking the expectation of a log is usually easier than the expectation
- We are allowed to choose the distribution to take the expectation over

– Ryan Adams[8]

[8] `Talking Machines Season 2, Episode 5`

Lower Bound[9]

$$\mathcal{L} = \int_{\mathbf{X},\mathbf{F}} q(\mathbf{X}) \log \left(\frac{p(\mathbf{Y}, \mathbf{F}, \mathbf{X})}{q(\mathbf{X})} \right)$$

[9] Damianou, A. C. (2015). Deep Gaussian Processes and Variational Propagation of Uncertainty (Doctoral dissertation)

Lower Bound[9]

$$\mathcal{L} = \int_{\mathbf{X},\mathbf{F}} q(\mathbf{X}) \log\left(\frac{p(\mathbf{Y},\mathbf{F},\mathbf{X})}{q(\mathbf{X})}\right)$$

$$\int_{\mathbf{X},\mathbf{F}} q(\mathbf{X}) \log\left(\frac{p(\mathbf{Y}|\mathbf{F})p(\mathbf{F}|\mathbf{X})p(\mathbf{X})}{q(\mathbf{X})}\right)$$

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$$\int_{\mathbf{X},\mathbf{F}} q(\mathbf{X}) \log \left(\frac{p(\mathbf{Y}|\mathbf{F}) p(\mathbf{F}|\mathbf{X}) p(\mathbf{X})}{q(\mathbf{X})} \right)$$

$$= \int_{\mathbf{F},\mathbf{X}} q(\mathbf{X}) \log p(\mathbf{Y}|\mathbf{F}) p(\mathbf{F}|\mathbf{X}) - \int_{\mathbf{X}} q(\mathbf{X}) \log \frac{q(\mathbf{X})}{p(\mathbf{X})}$$

[9] Damianou, A. C. (2015). Deep Gaussian Processes and Variational Propagation of Uncertainty (Doctoral dissertation)

Lower Bound[9]

$$
\begin{aligned}
\mathcal{L} = & \int_{\mathbf{X},\mathbf{F}} q(\mathbf{X}) \log \left(\frac{p(\mathbf{Y}, \mathbf{F}, \mathbf{X})}{q(\mathbf{X})} \right) \\
& \int_{\mathbf{X},\mathbf{F}} q(\mathbf{X}) \log \left(\frac{p(\mathbf{Y}|\mathbf{F}) p(\mathbf{F}|\mathbf{X}) p(\mathbf{X})}{q(\mathbf{X})} \right) \\
& = \int_{\mathbf{F},\mathbf{X}} q(\mathbf{X}) \log p(\mathbf{Y}|\mathbf{F}) p(\mathbf{F}|\mathbf{X}) - \int_{\mathbf{X}} q(\mathbf{X}) \log \frac{q(\mathbf{X})}{p(\mathbf{X})} \\
& = \tilde{\mathcal{L}} - \mathrm{KL}\left(q(\mathbf{X}) \parallel p(\mathbf{X})\right)
\end{aligned}
$$

[9] Damianou, A. C. (2015). Deep Gaussian Processes and Variational Propagation of Uncertainty (Doctoral dissertation)

Lower Bound

$$\tilde{\mathcal{L}} = \int_{\mathbf{F},\mathbf{X}} q(\mathbf{X}) \log p(\mathbf{Y}|\mathbf{F})p(\mathbf{F}|\mathbf{X})$$

- Has not eliviate the problem at all, X still needs to go through F to reach the data
- Idea of sparse approximations[10]

[10]Quinonero-Candela, Joaquin, & Rasmussen, C. E. (2005). A unifying view of sparse approximate Gaussian process regression & Snelson, E., & Ghahramani, Z. (2006). Sparse Gaussian processes using pseudo-inputs

Lower Bound

- Add another set of samples from the same prior

$$p(\mathbf{U}|\mathbf{Z}) = \prod_{j=1}^{d} \mathcal{N}(\mathbf{u}_{:,j}|\mathbf{0}, \mathbf{K})$$

Lower Bound

- Add another set of samples from the same prior

$$p(\mathbf{U}|\mathbf{Z}) = \prod_{j=1}^{d} \mathcal{N}(\mathbf{u}_{:,j}|\mathbf{0}, \mathbf{K})$$

- Conditional distribution

$$p(\mathbf{f}_{:,j}, \mathbf{u}_{:,j}|\mathbf{X}, \mathbf{Z}) = p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z})p(\mathbf{u}_{:,j}|\mathbf{Z})$$

$$= \mathcal{N}\left(\mathbf{f}_{:,j}|\mathbf{K}_{fu}(\mathbf{K}_{uu})^{-1}\mathbf{u}_{:,j}, \mathbf{K}_{ff} - \mathbf{K}_{fu}(\mathbf{K}_{uu})^{-1}\mathbf{K}_{uf}\right)\mathcal{N}\left(\mathbf{u}_{:,j}|\mathbf{0}, \mathbf{K}_{uu}\right),$$

Lower Bound

$$p(\mathbf{Y}, \mathbf{F}, \mathbf{U}, \mathbf{X}|\mathbf{Z}) = p(\mathbf{X}) \prod_{j=1}^{d} p(\mathbf{y}_{:,j}|\mathbf{f}_{:,j}) p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}) p(\mathbf{u}_{:,j}|\mathbf{Z})$$

- we have done nothing to the model, just added *halucinated* observations

Lower Bound

$$p(\mathbf{Y}, \mathbf{F}, \mathbf{U}, \mathbf{X}|\mathbf{Z}) = p(\mathbf{X}) \prod_{j=1}^{d} p(\mathbf{y}_{:,j}|\mathbf{f}_{:,j}) p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}) p(\mathbf{u}_{:,j}|\mathbf{Z})$$

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- however, we will now interpret $\mathbf{U}$ and $\mathbf{X}_u$ not as random variables but variational parameters

Lower Bound

$$p(\mathbf{Y}, \mathbf{F}, \mathbf{U}, \mathbf{X}|\mathbf{Z}) = p(\mathbf{X}) \prod_{j=1}^{d} p(\mathbf{y}_{:,j}|\mathbf{f}_{:,j}) p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}) p(\mathbf{u}_{:,j}|\mathbf{Z})$$

- we have done nothing to the model, just added *halucinated* observations
- however, we will now interpret $\mathbf{U}$ and $\mathbf{X}_u$ not as random variables but variational parameters
- i.e. parametrise approximate posterior using these parameters (remember sparse motivation)

Lower Bound

- Variational distributions are approximations to intractable posteriors,

$$
\begin{aligned}
q(\mathbf{U}) &\approx p(\mathbf{U}|\mathbf{Y}, \mathbf{X}, \mathbf{Z}, \mathbf{F}) \\
q(\mathbf{F}) &\approx p(\mathbf{F}|\mathbf{U}, \mathbf{X}, \mathbf{Z}, \mathbf{Y}) \\
q(\mathbf{X}) &\approx p(\mathbf{X}|\mathbf{Y})
\end{aligned}
$$

Lower Bound

- Variational distributions are approximations to intractable posteriors,

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

- Assume that we can *find* **U** that completely represents **F**, i.e. **U** is sufficient statistics of **F**,

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

Lower Bound

$$\tilde{\mathcal{L}} = \int_{\mathbf{X},\mathbf{F},\mathbf{U}} q(\mathbf{F})q(\mathbf{U})q(\mathbf{X}) \log \frac{p(\mathbf{Y},\mathbf{F},\mathbf{U}|\mathbf{X},\mathbf{Z})}{q(\mathbf{F})q(\mathbf{U})}$$

Lower Bound

$$\tilde{\mathcal{L}} = \int_{\mathbf{X},\mathbf{F},\mathbf{U}} q(\mathbf{F})q(\mathbf{U})q(\mathbf{X}) \log \frac{p(\mathbf{Y},\mathbf{F},\mathbf{U}|\mathbf{X},\mathbf{Z})}{q(\mathbf{F})q(\mathbf{U})}$$

$$= \int_{\mathbf{X},\mathbf{F},\mathbf{U}} q(\mathbf{F})q(\mathbf{U})q(\mathbf{X}) \log \frac{\prod_{j=1}^{d} p(\mathbf{y}_{:,j}|\mathbf{f}_{:,j})p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j},\mathbf{X},\mathbf{Z})p(\mathbf{u}_{:,j}|\mathbf{Z})}{q(\mathbf{F})q(\mathbf{U})}$$

Lower Bound

$$\tilde{\mathcal{L}} = \int_{\mathbf{X},\mathbf{F},\mathbf{U}} q(\mathbf{F})q(\mathbf{U})q(\mathbf{X}) \log \frac{p(\mathbf{Y},\mathbf{F},\mathbf{U}|\mathbf{X},\mathbf{Z})}{q(\mathbf{F})q(\mathbf{U})}$$

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- Assume that $\mathbf{U}$ is sufficient statistics for $\mathbf{F}$

$$q(\mathbf{F})q(\mathbf{U})q(\mathbf{X}) = p(\mathbf{F}|\mathbf{U},\mathbf{X},\mathbf{Z})q(\mathbf{U})q(\mathbf{X})$$

Lower Bound

$$\tilde{\mathcal{L}} = \int_{\mathbf{X},\mathbf{F},\mathbf{U}} \prod_{j=1}^{d} p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}_{:,j}) q(\mathbf{X})$$

$$\log \frac{\prod_{j=1}^{d} p(\mathbf{y}_{:,j}|\mathbf{f}_{:,j}) p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z}) p(\mathbf{u}_{:,j}|\mathbf{Z})}{\prod_{j=1}^{d} p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}_{:,j})} =$$

Lower Bound

$$\tilde{\mathcal{L}} = \int_{\mathbf{X},\mathbf{F},\mathbf{U}} \prod_{j=1}^{d} p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}_{:,j}) q(\mathbf{X})$$

$$\log \frac{\prod_{j=1}^{d} p(\mathbf{y}_{:,j}|\mathbf{f}_{:,j}) p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z}) p(\mathbf{u}_{:,j}|\mathbf{Z})}{\prod_{j=1}^{d} p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}_{:,j})} =$$

$$= \int_{\mathbf{X},\mathbf{F},\mathbf{U}} \prod_{j=1}^{p} p(\mathbf{f}_{:,j}|\mathbf{u}_{:,j}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}_{:,j}) q(\mathbf{X}) \log \frac{\prod_{j=1}^{p} p(\mathbf{y}_{:,j}|\mathbf{f}_{:,j}) p(\mathbf{u}_{:,j}|\mathbf{Z})}{\prod_{j=1}^{p} q(\mathbf{u}_{:,j})}$$

$$= \mathbb{E}_{q(\mathbf{F}),q(\mathbf{X}),q(\mathbf{U})} \left[p(\mathbf{Y}|\mathbf{F}) \right] - \mathrm{KL}\left(q(\mathbf{U}) || p(\mathbf{U}|\mathbf{Z}) \right)$$

Summary

$$\mathbb{E}_{q(\mathbf{F}),q(\mathbf{X}),q(\mathbf{U})}\left[p(\mathbf{Y}|\mathbf{F})\right] - \mathrm{KL}\left(q(\mathbf{U})||p(\mathbf{U}|\mathbf{Z})\right) - \mathrm{KL}\left(q(\mathbf{X})||p(\mathbf{X})\right)$$

- Expectation tractable (for some co-variances)
- Reduces to expectations over co-variance functions know as Ψ statistics
- Allows us to place priors and not "regularisers" over the latent representation

Latent space priors

Latent space priors[11]

$$\mathbb{E}_{q(\mathbf{F}),q(\mathbf{X}),q(\mathbf{U})}\left[p(\mathbf{Y}|\mathbf{F})\right] - \mathrm{KL}\left(q(\mathbf{U})||p(\mathbf{U}|\mathbf{Z})\right) - \mathrm{KL}\left(q(\mathbf{X})||p(\mathbf{X})\right)$$

- Importantly $p(\mathbf{X})$ appears only in KL term
- Allows us to express stronger assumptions about the model

[11] Damianou, A. C., Titsias, M., & Lawrence, Neil D, Variational Inference for Uncertainty on the Inputs of Gaussian Process Models (2014)

Non-Gaussian Data

Theorem (Change-of-variable)

$$p_y(y) = p_x(\rho(y))|\nabla\rho(y)|$$

$$x \in \mathcal{X} \subseteq R^{D_x} \quad y \in \mathcal{Y} \subseteq R^{D_y}$$

- $\rho : \mathcal{Y} \to \mathcal{X}$
- ρ *is a bijective function*

Change of Variables

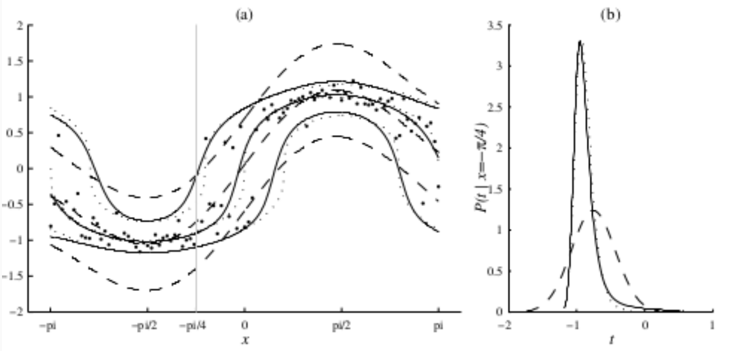
$$p(y) = \mathcal{N}(\rho(y)\mu, \Sigma)|\nabla\rho(y)| \quad p(y_*|y) = \mathcal{N}(\rho(y)|\mu(x_*|x), \Sigma(x_*|x))|\nabla\rho(y)|$$

$$p(x) \sim \mathcal{N}(\mu, \Sigma) \quad p(x_*|x) = \mathcal{N}(\rho(y)|\mu(x_*|x), \Sigma(x_*|x))$$

Change of Variable

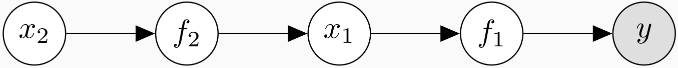
- We can model non-gaussian data y using a Gaussian variable x if we have a transformation ρ that makes it "Gaussian"

Warped Gaussian Processes[12, 13]



[12]Snelson, E., & Ghahramani, Z. (2004). Warped Gaussian Processes
[13]Lazaro-Gredilla, Miguel (2012). Bayesian Warped Gaussian Processes. In , Advances in Neural Information Processing Systems

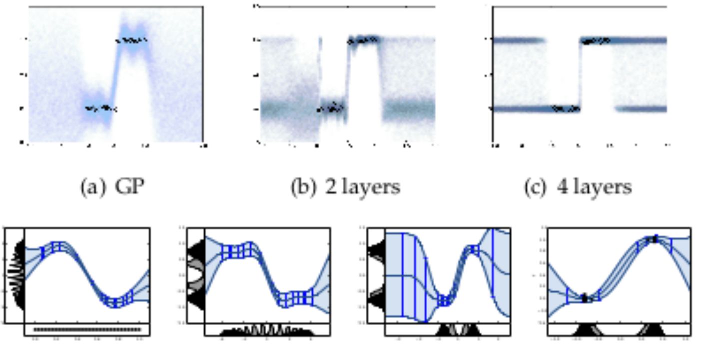
Deep Gaussian Processes[14]



- Place a GP as a warping function, that is warped, ...

[14] Damianou, A. C., & Lawrence, N. D. (2013). Deep Gaussian Processes

Deep Gaussian Processes[15]

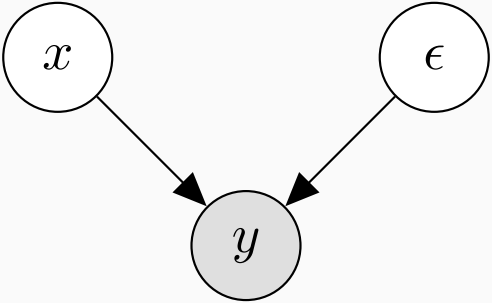


(a) GP (b) 2 layers (c) 4 layers

(d) Hidden spaces for 4 layer model

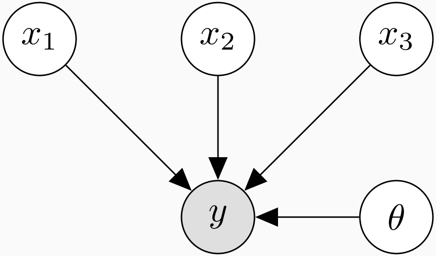
[15] *Stolen from Neil, who borrowed it from James, who we believe genereated the plot*

Explaining Away



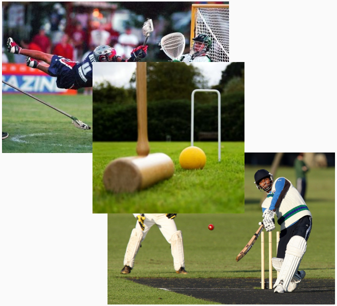
$$y = f(x) + \epsilon$$

Factor Analysis

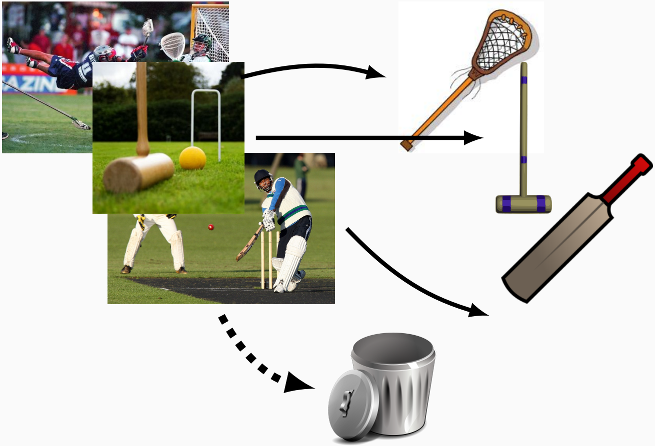


$$y = f(x_1, x_2, x_3) + \epsilon$$

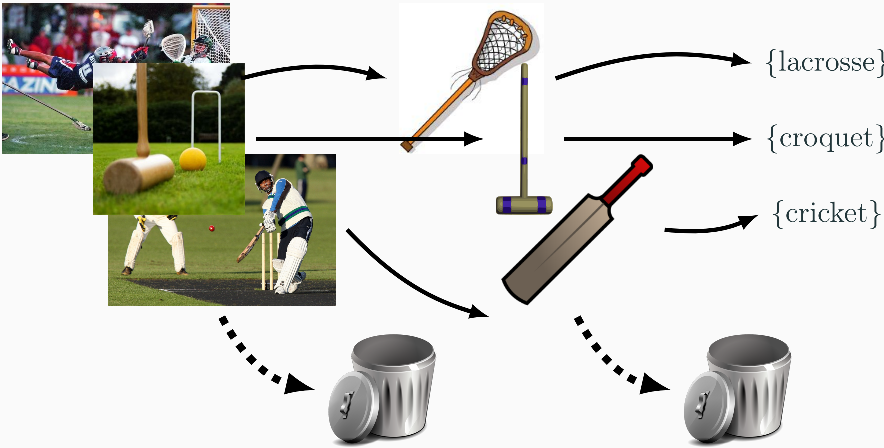
Latent Structure



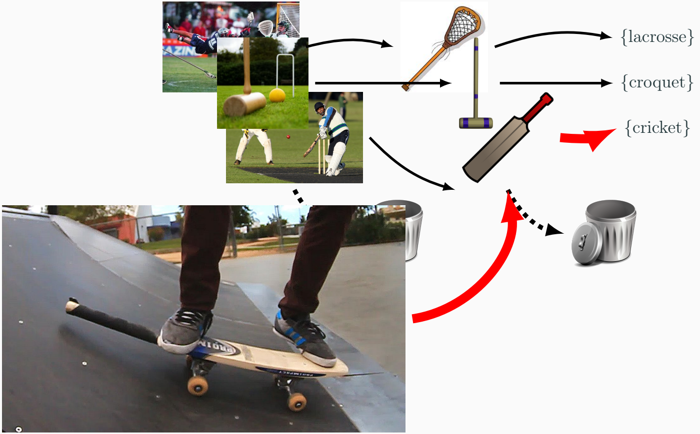
Latent Structure



Latent Structure

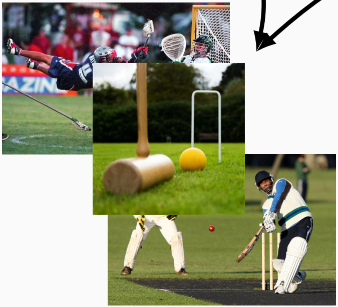


Latent Structure

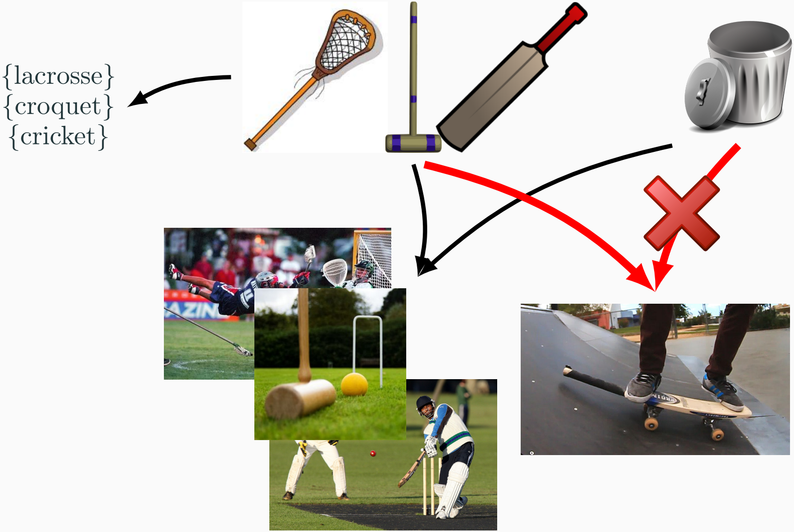


Latent Structure

$\{\text{lacrosse}\}$
$\{\text{croquet}\}$
$\{\text{cricket}\}$

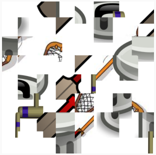


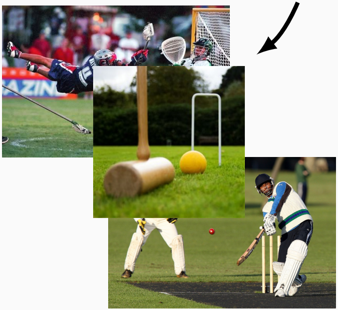
Latent Structure



Latent Structure

{lacrosse}
{croquet}
{cricket}





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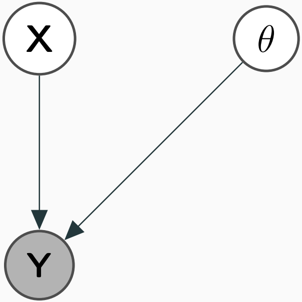
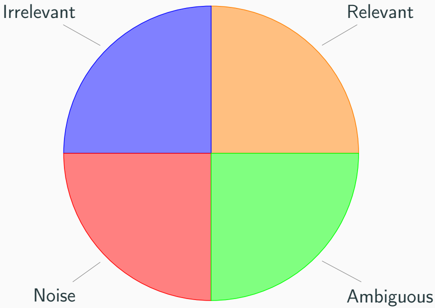
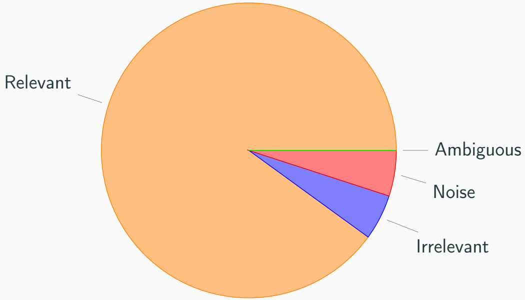


Latent Structure



Latent Structure



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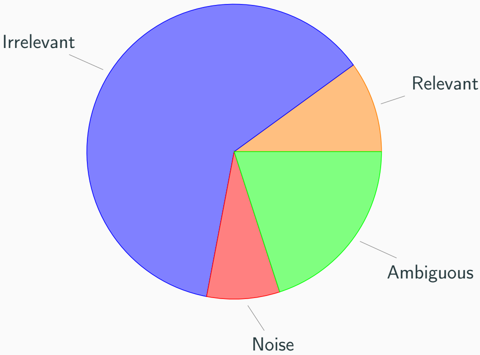
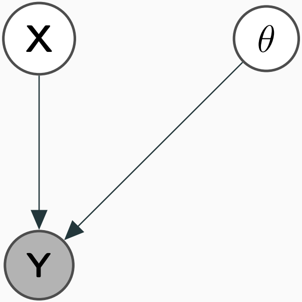
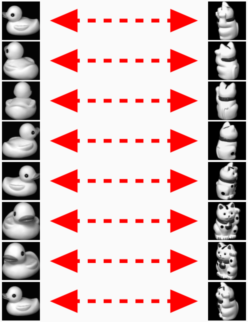


Latent Structure

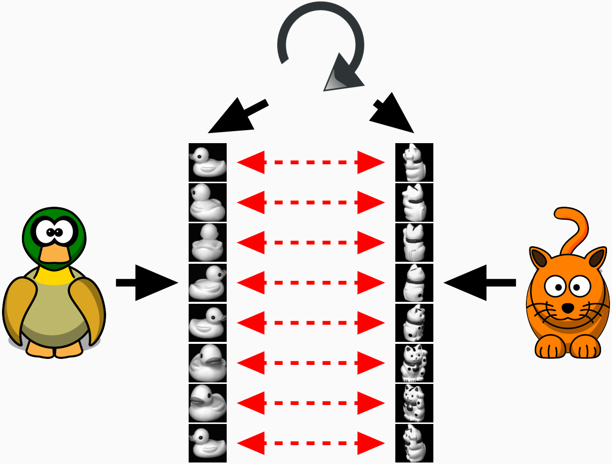


Alignments

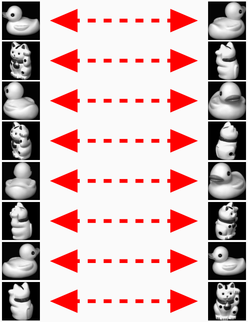
Alignments



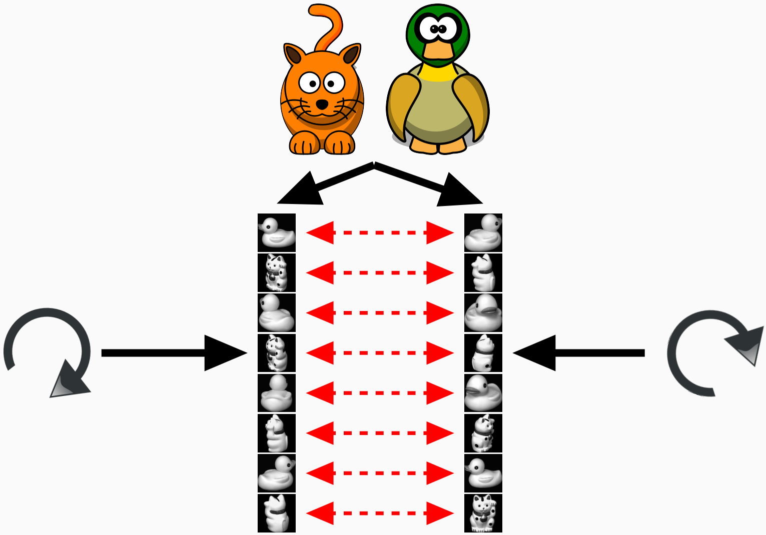
Alignments



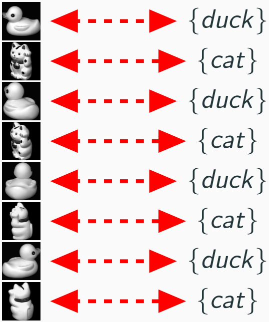
Alignments



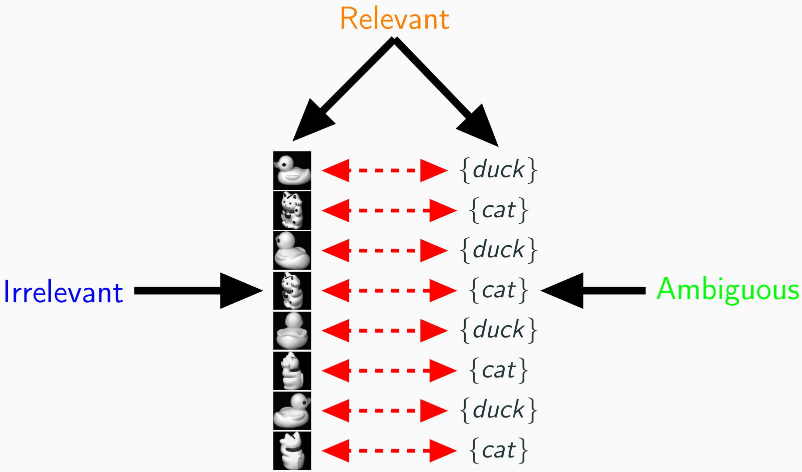
Alignments



Alignments



Alignments


Relevant
Irrelevant
Ambiguous
$\{duck\}$
$\{cat\}$
$\{duck\}$
$\{cat\}$
$\{duck\}$
$\{cat\}$
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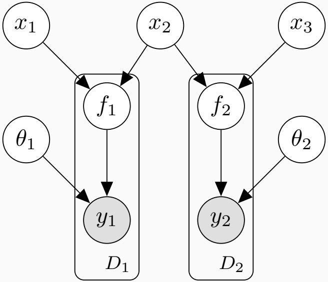
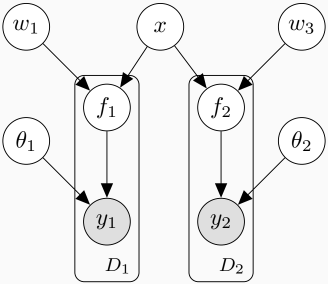
$\{cat\}$

Explaining Away cont.



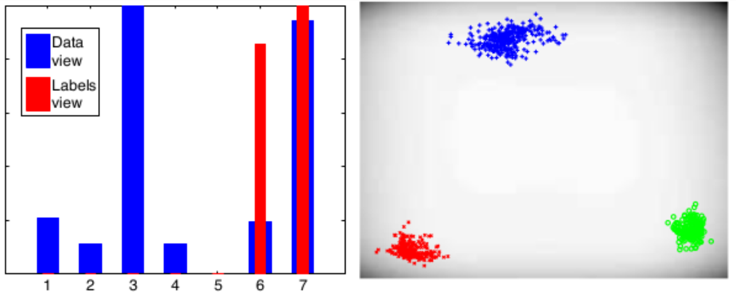
IBFA with GP-LVM[16]



$$y_1 = f(w_1^{\mathrm{T}} x) \quad y_2 = f(w_2^{\mathrm{T}} x)$$

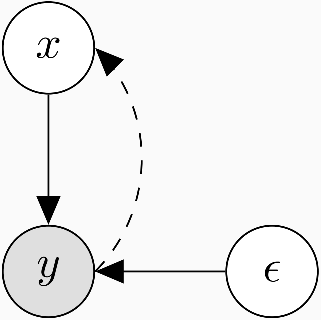
[16]Damianou, A., Lawrence, N. D., & Ek, C. H. (2016). Multi-view learning as a nonparametric nonlinear inter-battery factor analysis

IBFA with GP-LVM



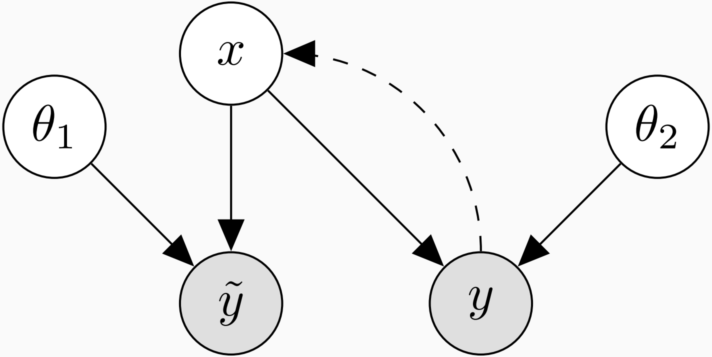
IBFA with GP-LVM

Constrained Latent Space



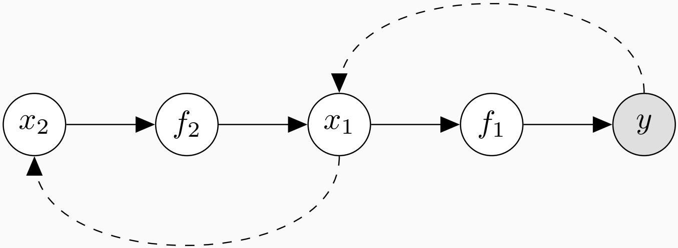
$$y = f(g(y)) + \epsilon$$

Denoising Auto-encoder[17, 18]



[17]Ek, C. H., Torr, P. H. S., & Lawrence, N. D., Gaussian process latent variable models for human pose estimation, International conference on Machine learning for multimodal interaction, (), 132–143 (2007).
[18]Snoek, J., Adams, R. P., & Larochelle, H., Nonparametric guidance of autoencoder representations using label information, Journal of Machine

VAE[19]



$$q(x_l) = g(x_{l-1})$$

[19]Dai, Z., Damianou, A., Gonz\'alez, Javier, & Lawrence, N., Variational auto-encoded deep Gaussian processes, International Conference on Learning Representations (ICLR), (2016).

Summary

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  - *Its actually not, its really really easy.*
- Relevant assumptions needed to learn anything useful
- Strong assumptions needed to learn anything from "sensible" amounts of data
- GPs provide strong, interpretative assumptions that aligns well to our intuitions allowing us to make relevant assumptions

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