Machine Learning and the Physical World

Lecture 4 : Inference and Latent Variables

Carl Henrik Ek - che29@cam.ac.uk

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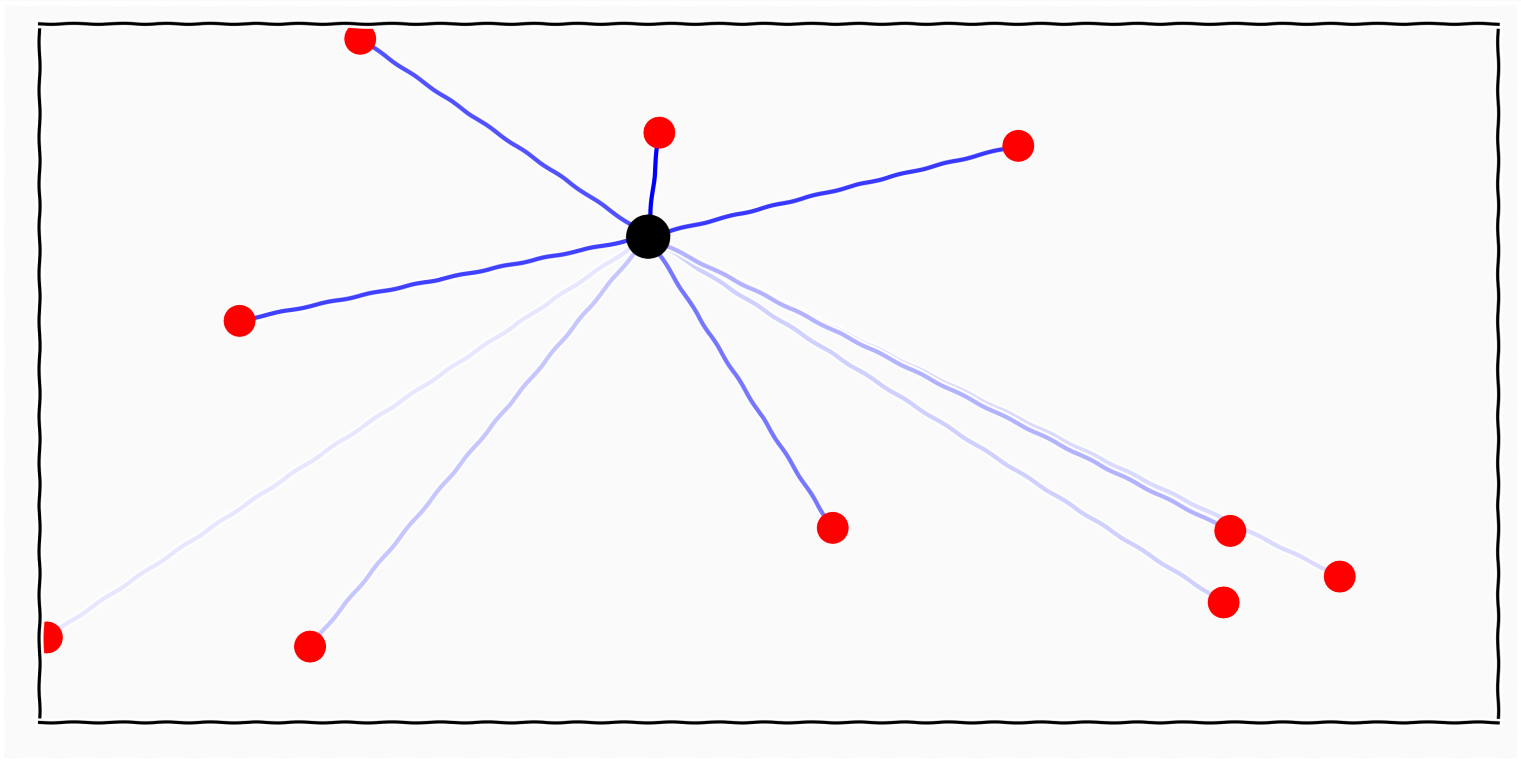
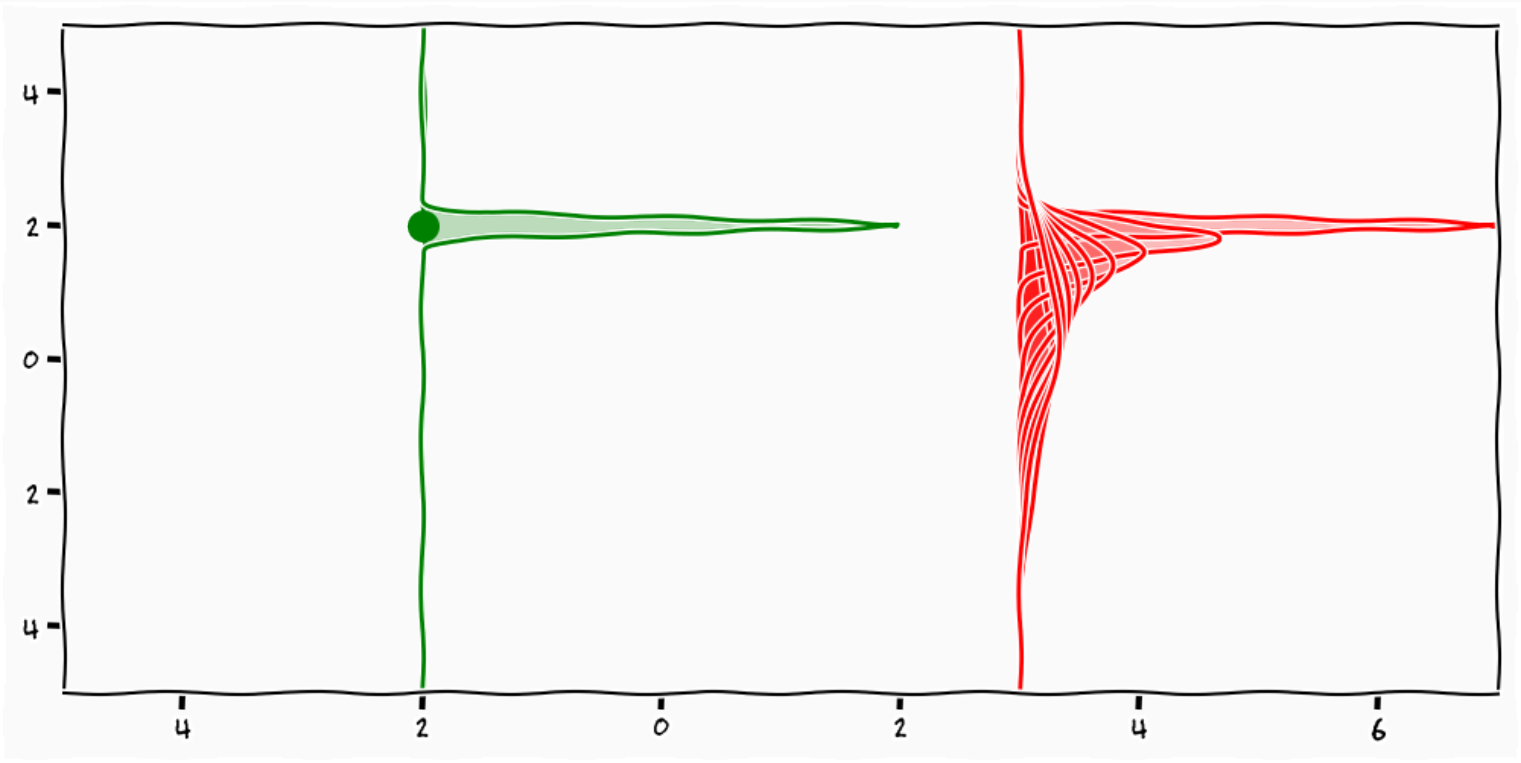
http://carlhenrik.com

Non-parametrics



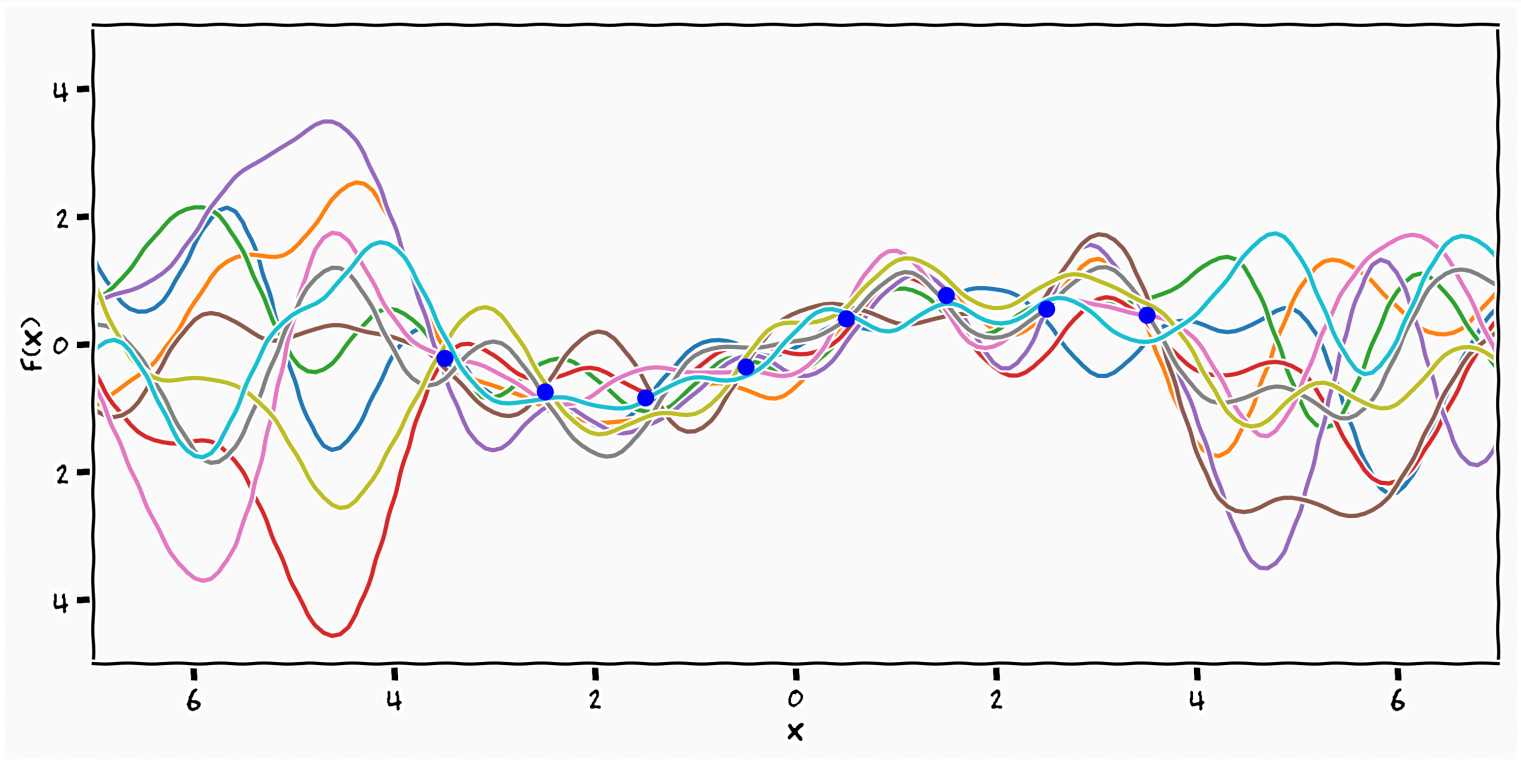
Non-parametric functions



Gaussian Processes: Formalism II

$$p(\mathbf{f}) = \mathcal{N}\left(\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \\ \vdots \end{bmatrix} \middle\| \begin{bmatrix} \mu(x_1) \\ \mu(x_2) \\ \vdots \\ \mu(x_N) \\ \vdots \end{bmatrix}, \begin{bmatrix} k(x_1,x_1) & k(x_1,x_2) & \dots & k(x_1,x_N) & \dots \\ k(x_2,x_1) & k(x_2,x_2) & \dots & k(x_2,x_N) & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ k(x_N,x_1) & k(x_N,x_2) & \dots & k(x_N,x_N) & \dots \\ \vdots & \vdots & \dots & \vdots & \ddots \end{bmatrix}\right)$$

Posterior Samples



Gaussian processes

$$\mathcal{GP}(\cdot,\cdot) \qquad M \in \mathbb{R}^{\infty \times N} \qquad \mathcal{N}(\cdot,\cdot)$$

$$\infty \qquad \rightarrow \qquad N$$

The Gaussian distribution is the projection of the infinite Gaussian process

Predictive Posteriors

- Gaussian Process - *Non-parametric formulation*

$$
\begin{aligned}
p(y_* \mid \mathbf{y}, \mathbf{x}_*, \mathbf{X}, \theta) &= \mathcal{N}(y_* \mid \mu_*, K_*) \\
\mu_* &= k(x_*, x)k(x, x)^{-1}\mathbf{y} \\
K_* &= k(x_*, x_*) - k(x_*, x)k(x, x)^{-1}k(x, x_*)
\end{aligned}
$$

Predictive Posteriors

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$$

- Linear Regression - *Parametric formulation*

$$
\begin{aligned}
p(y_*|\mathbf{y}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) &= \int p(y_*|\mathbf{x}_*, \mathbf{w}, \beta)p(\mathbf{w}|\mathbf{y}, \mathbf{X}, \alpha, \beta)\mathrm{d}\mathbf{w} \\
&= \mathcal{N}\left((y_* \mid \mu_*(x_*), \Sigma_*(x_*)\right) \\
\mu_* &= \left(\beta(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})^{-1}\mathbf{x}\mathbf{y}\right)^{\mathrm{T}}\mathbf{x}_* \\
&= \mathbf{x}_*^{\mathrm{T}}\mathbf{x}\left(\beta(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})\right)^{-1}\mathbf{y} \\
\Sigma_* &= \frac{1}{\beta} + \mathbf{x}_*^{\mathrm{T}}(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})^{-1}\mathbf{x}
\end{aligned}
$$

Regression Models: Mean

$$k(x_*, x)k(x, x)^{-1}\mathbf{y} \qquad \mathbf{x}_*^{\mathrm{T}}\mathbf{x}\left(\beta(\alpha\mathbf{I} + \beta\mathbf{x}^{\mathrm{T}}\mathbf{x})\right)^{-1}\mathbf{y}$$

- both means are linear with respect to the output data

Regression Models: Mean

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- if we think of $\mathbf{x}$ as the center of each basis function

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- if we could parametrise $\Phi(\mathbf{x}_*)^{\mathrm{T}}\Phi(\mathbf{x}) = k(\mathbf{x}_*, \mathbf{x})$ as a function

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- if we could parametrise $\Phi(\mathbf{x}_*)^{\mathrm{T}}\Phi(\mathbf{x}) = k(\mathbf{x}_*, \mathbf{x})$ as a function
- this leads to the interpretation of GPs as infinite basis functions

The Marginal Likelihood

Semantics

$$p(\theta \mid y) = \frac{p(y \mid \theta)p(\theta)}{\int p(y \mid \theta)p(\theta)\mathrm{d}\theta}$$

Likelihood How much evidence is there in the data for a specific hypothesis

Prior What are my beliefs about different hypothesis

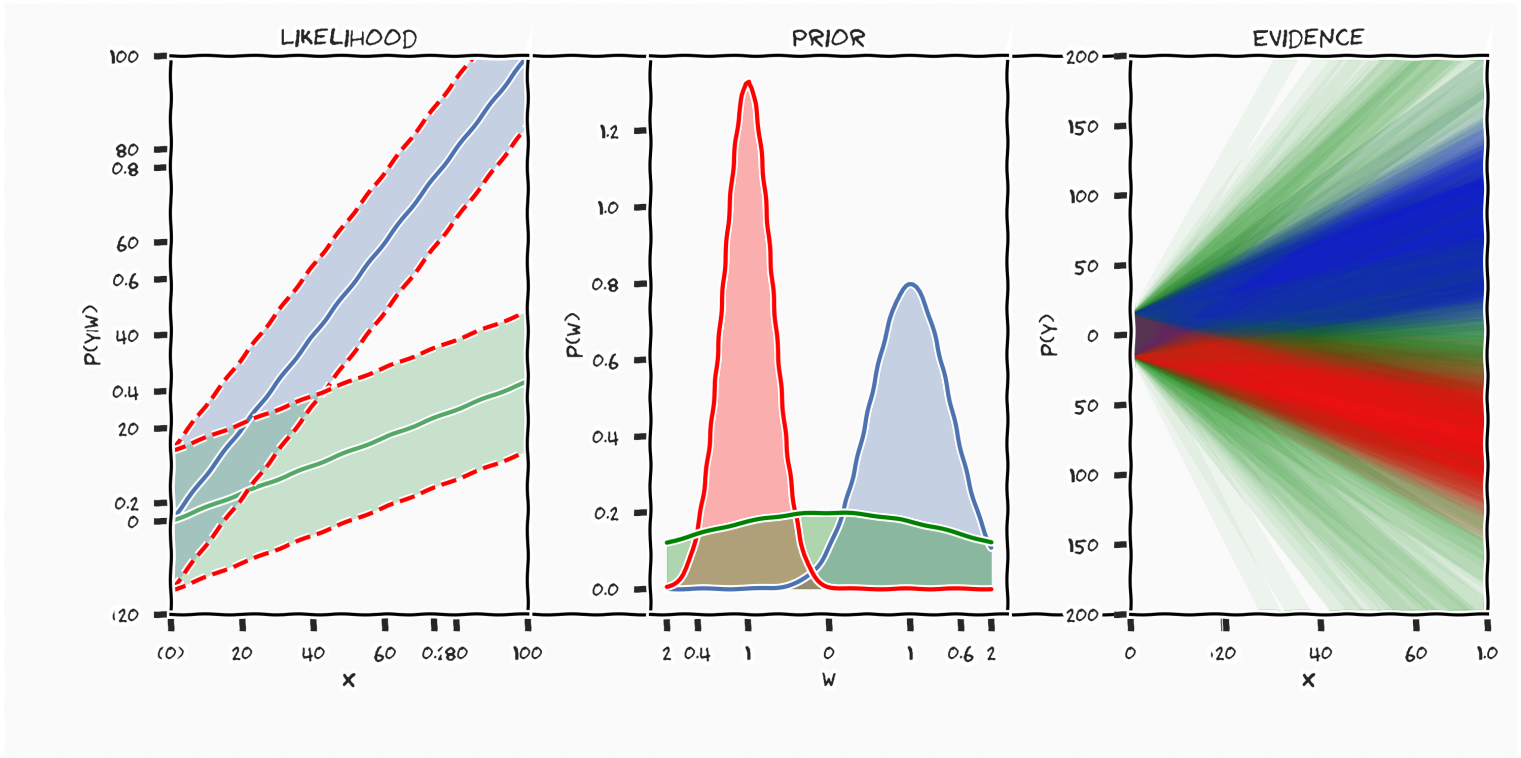
Posterior What is my updated belief after having seen data

Evidence What is my belief about the data

The Compute: Evidence

$$\int p(y \mid \theta) p(\theta) \mathrm{d}\theta$$

Regression Model



Marginalisation

Next time you want to give your friends a compliment, tell them that you have completely marginalised them from your life

Regression Models

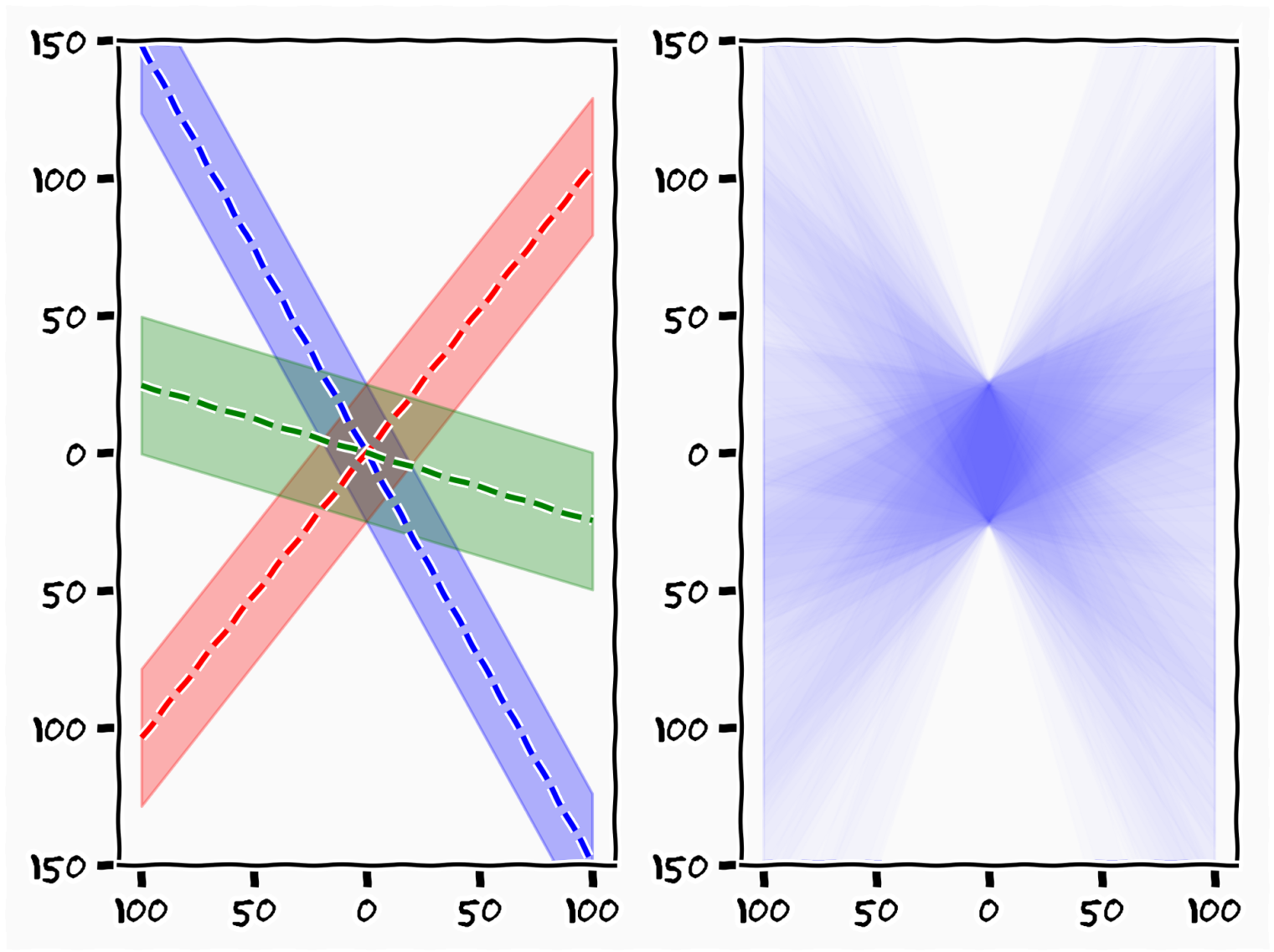
Linear Linear Model

$$p(y_i|x_i, \mathbf{w}) = \mathcal{N}(w_0 + w_1 \cdot x_i, \beta^{-1})$$

Basis function

$$p(y_i|x_i, \mathbf{w}) = \mathcal{N}(\sum_{i=1}^{6} w_i \phi(x_i), \beta^{-1})$$

Model 1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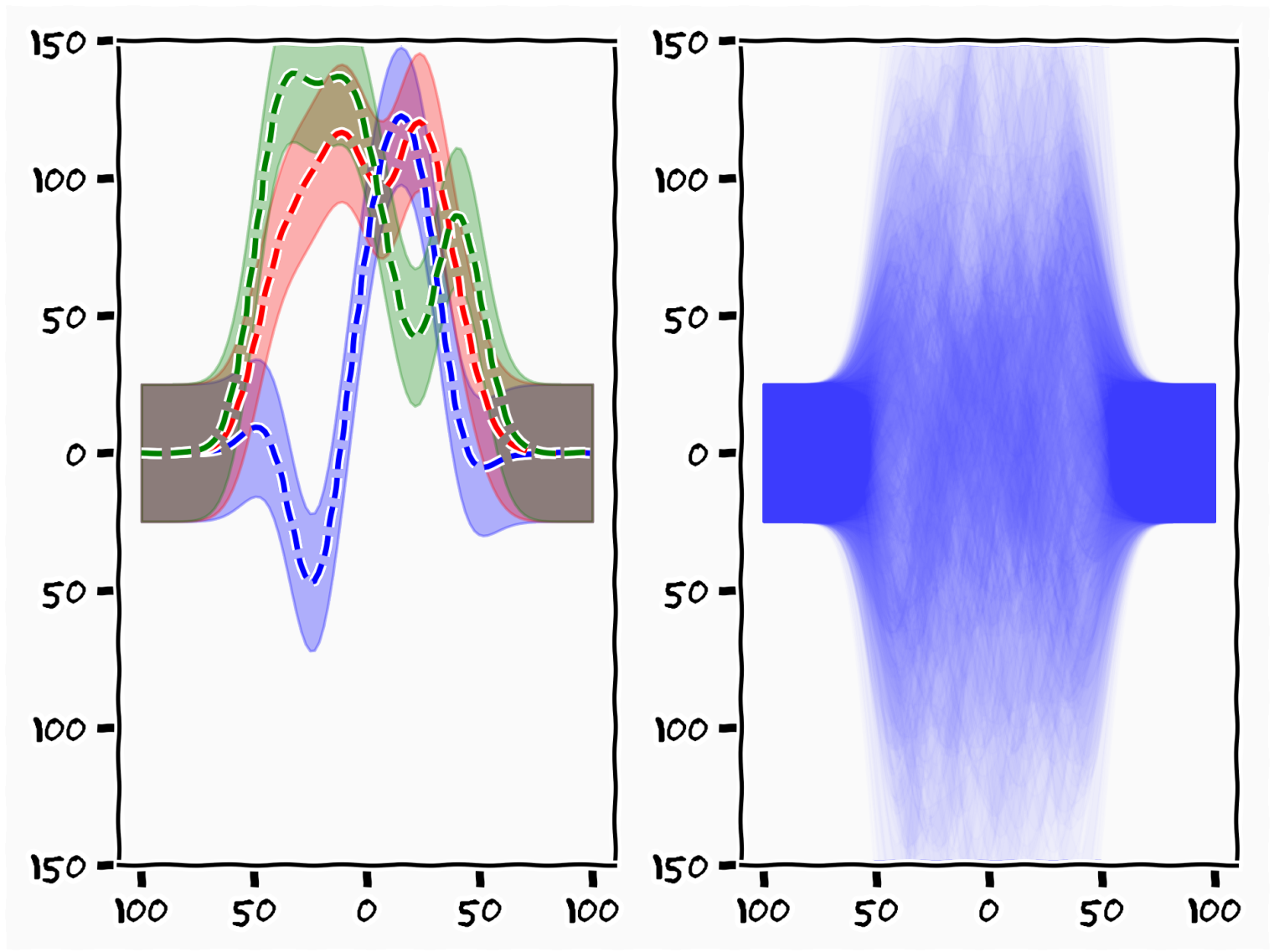
Model 2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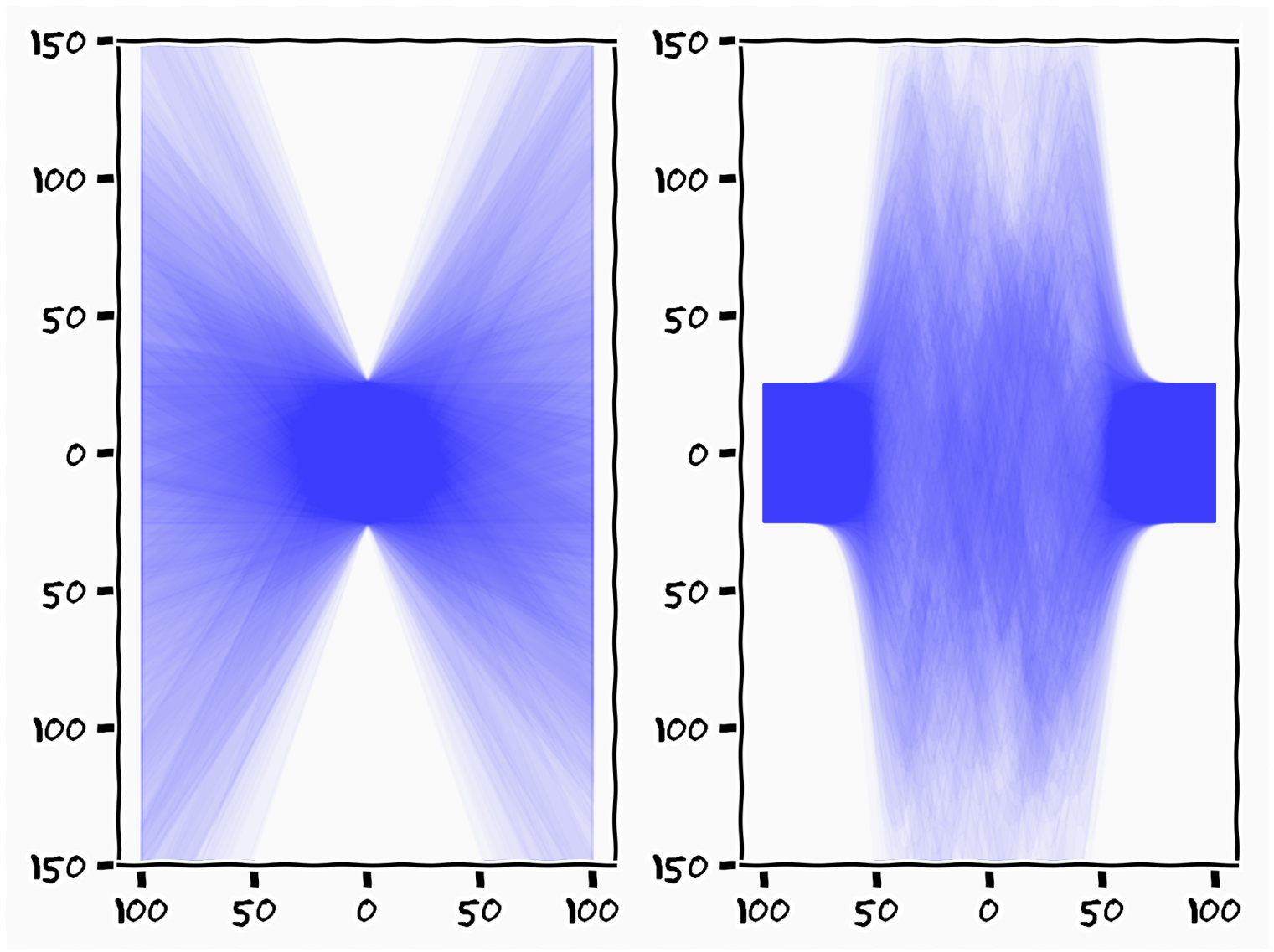
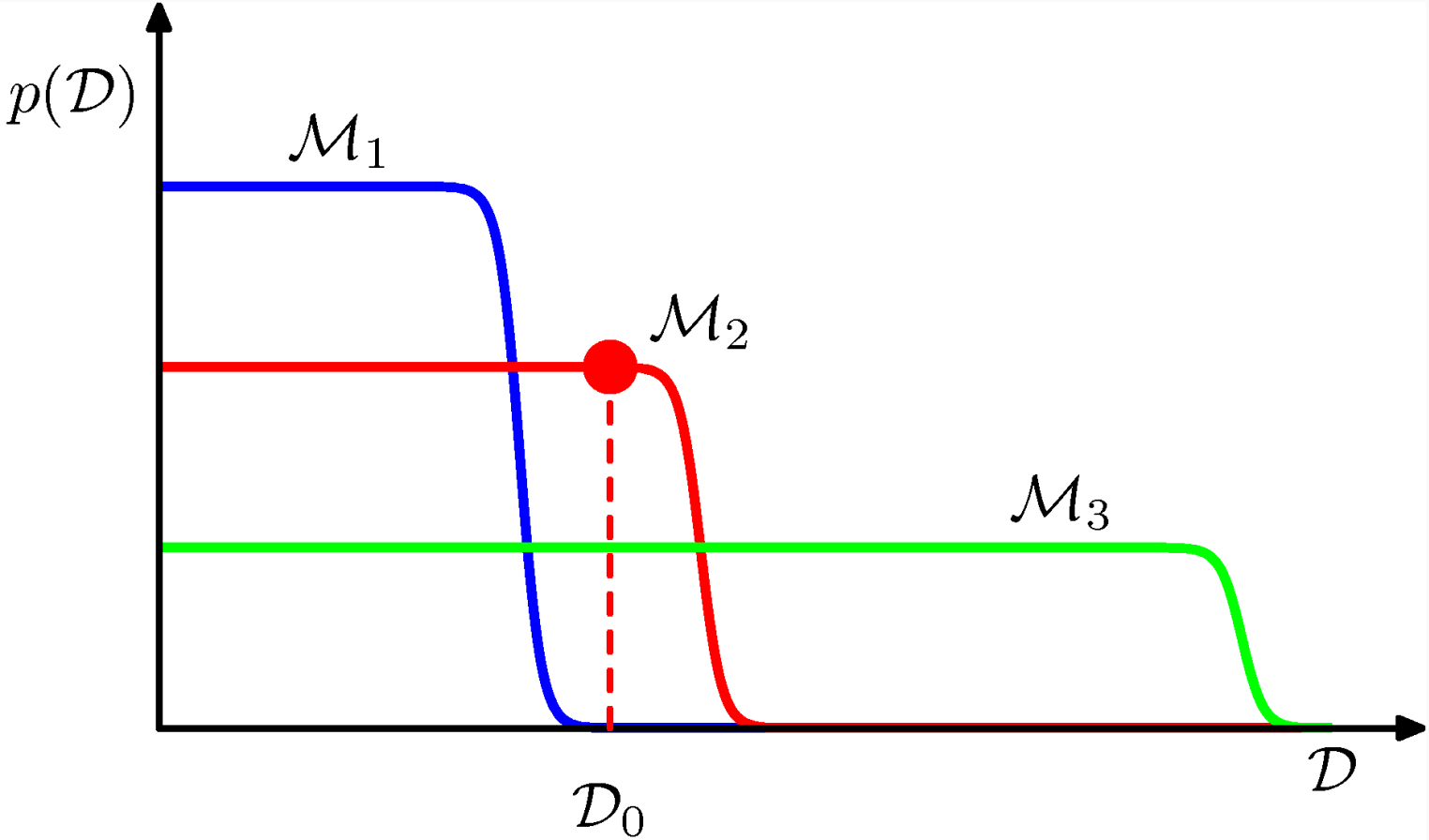
Evidence



Probabilities are a zero-sum game

Model Selection[1]



[1] David MacKay PhD Thesis

Occams Razor

Occams Razor

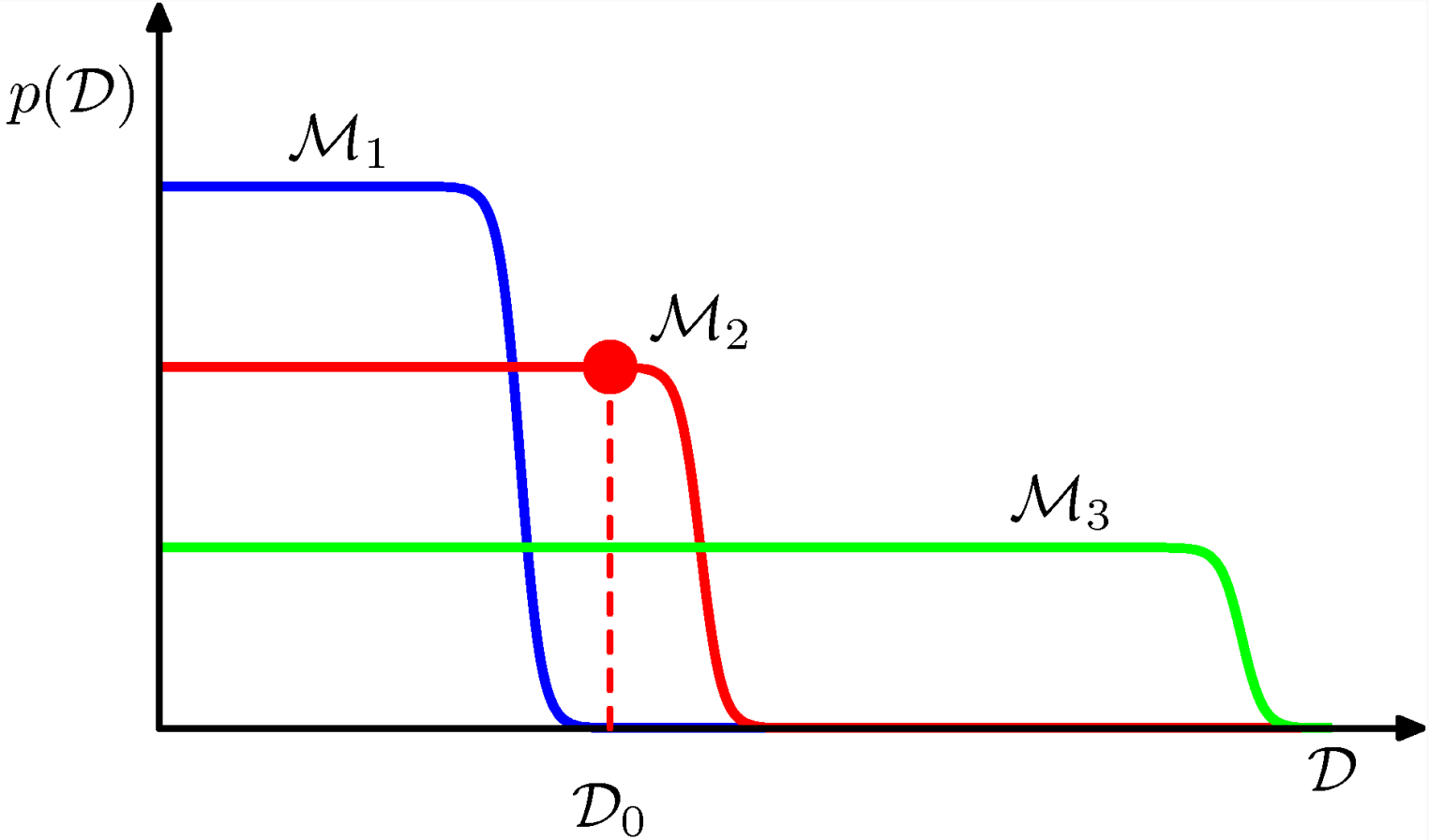
Definition (Occams Razor)
"All things being equal, the simplest solution tends to be the best one"

– William of Ockham

What is Simple?[2]

[2] https://www.imdb.com/title/tt8132700/

Model Selection[1]



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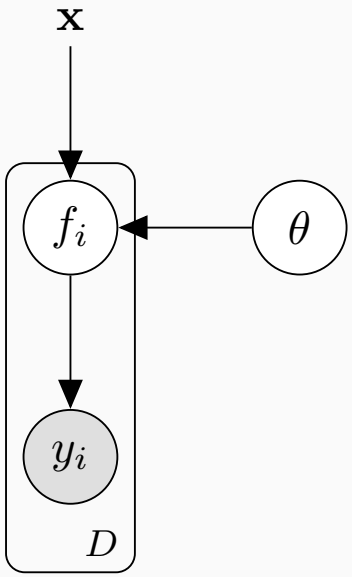
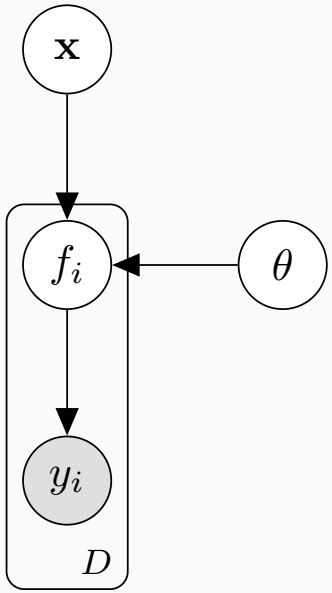
The Compute: Evidence

$$\int p(y \mid \theta) p(\theta) \mathrm{d}\theta$$

Unsupervised Learning



$p(y|x)$



$p(y)$

Gaussian Process Latent Variable Model [3]

- Regression

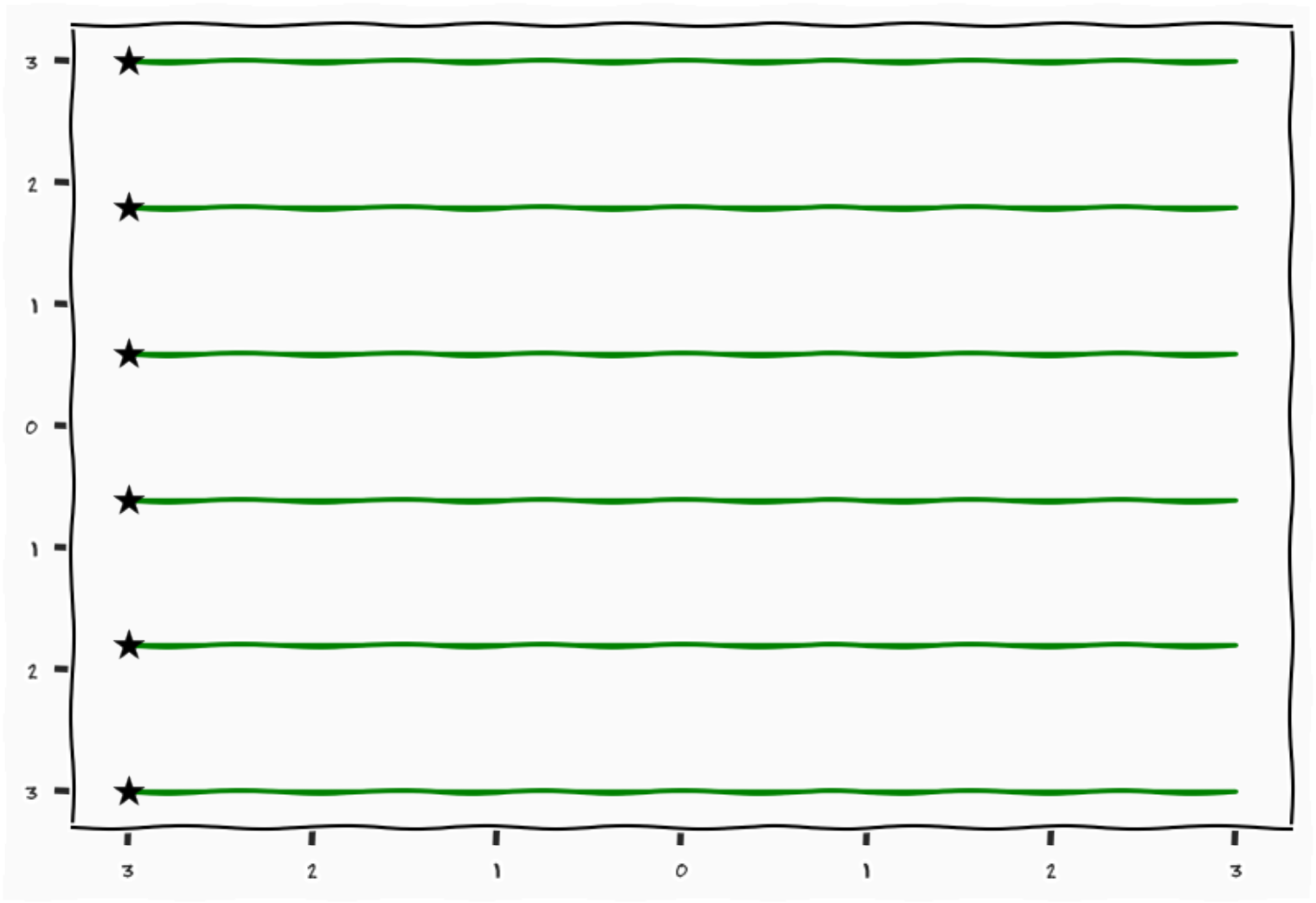
$$p(y \mid x) = \int p(y \mid f)p(f \mid x)\mathrm{d}f$$

- "Unsupervised" Learning

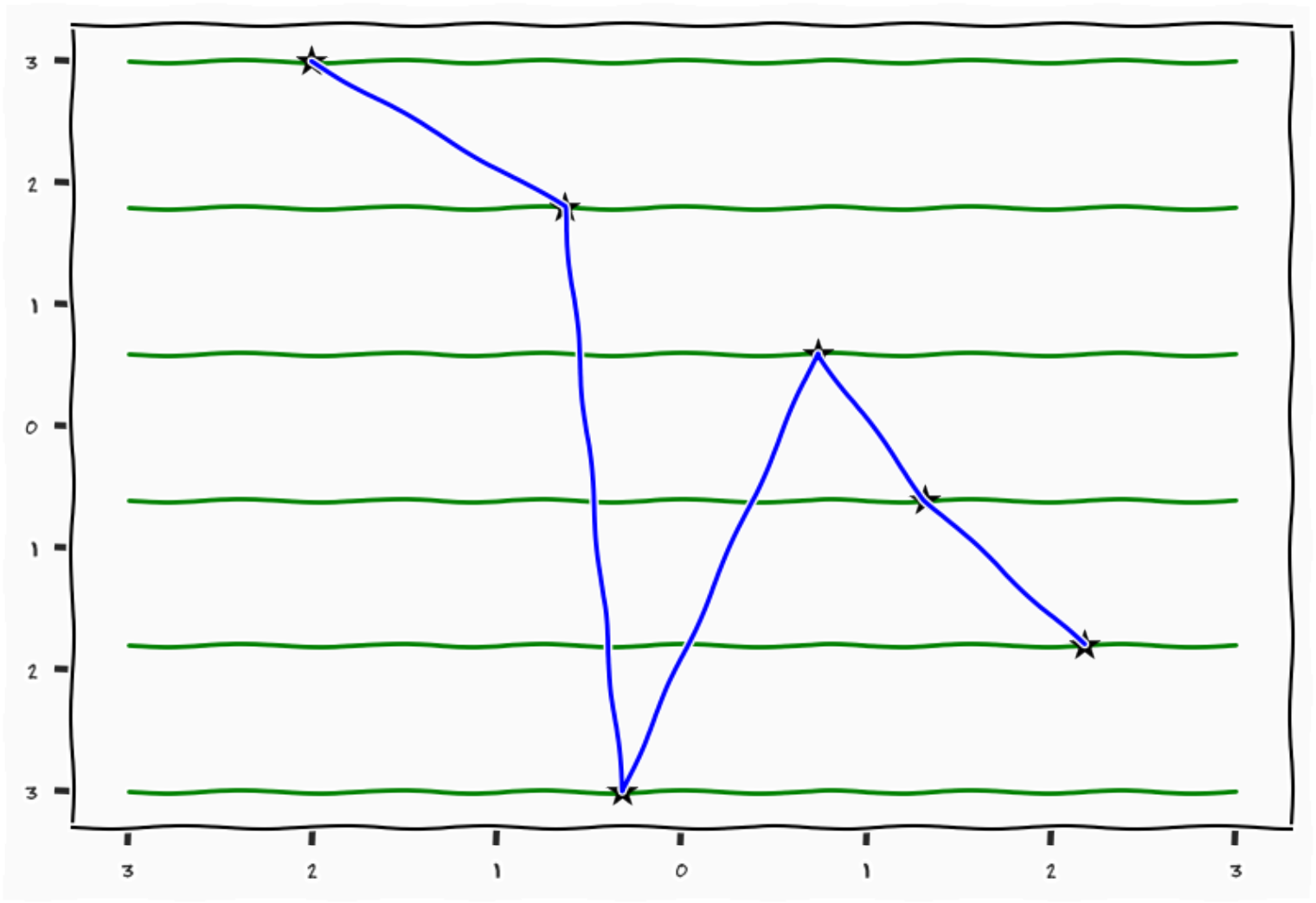
$$p(y) = \int p(y \mid f)p(f \mid x)p(x)\mathrm{d}f\mathrm{d}x$$

[3] Lawrence, 2005

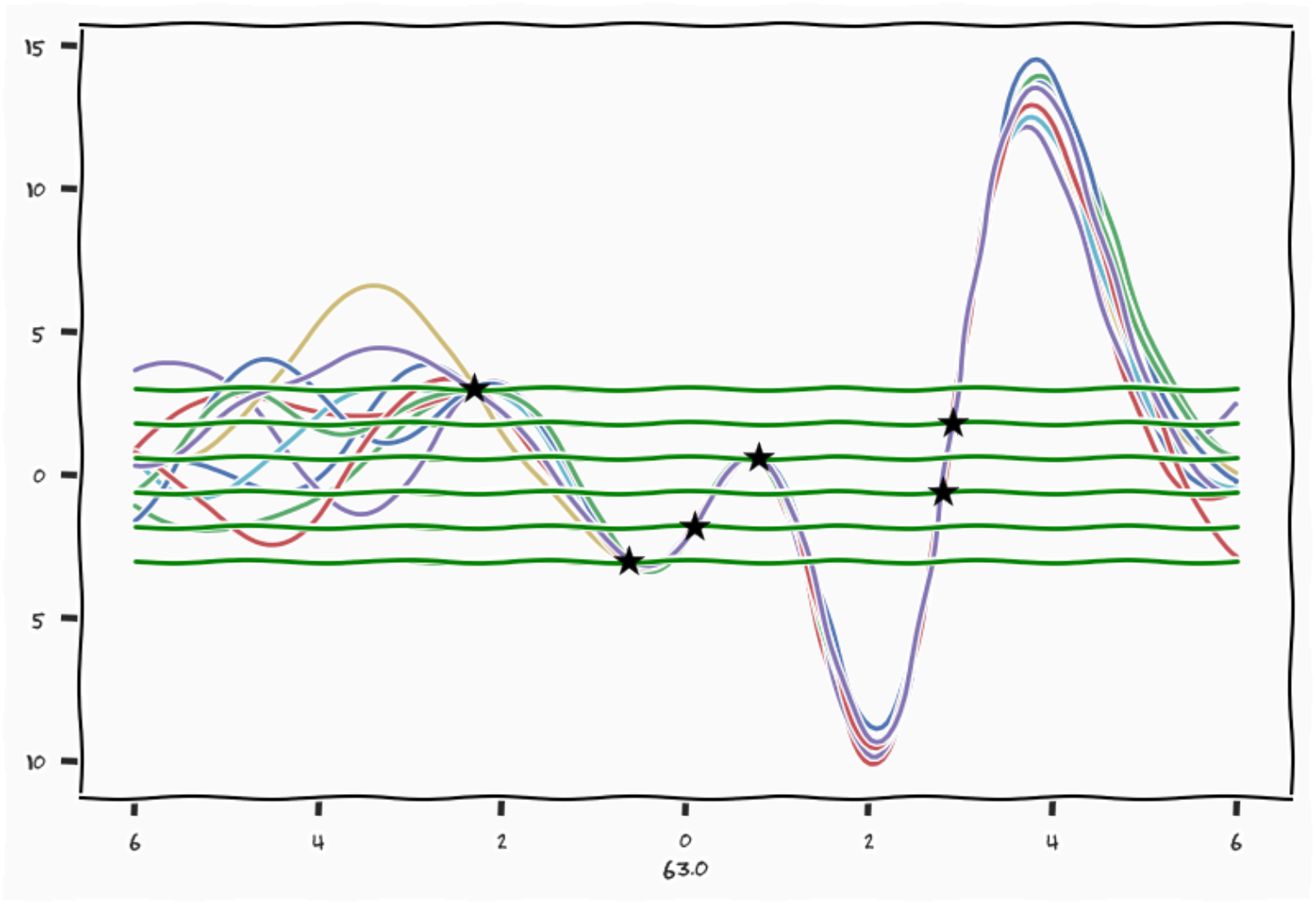
Unsupervised Learning



Unsupervised Learning

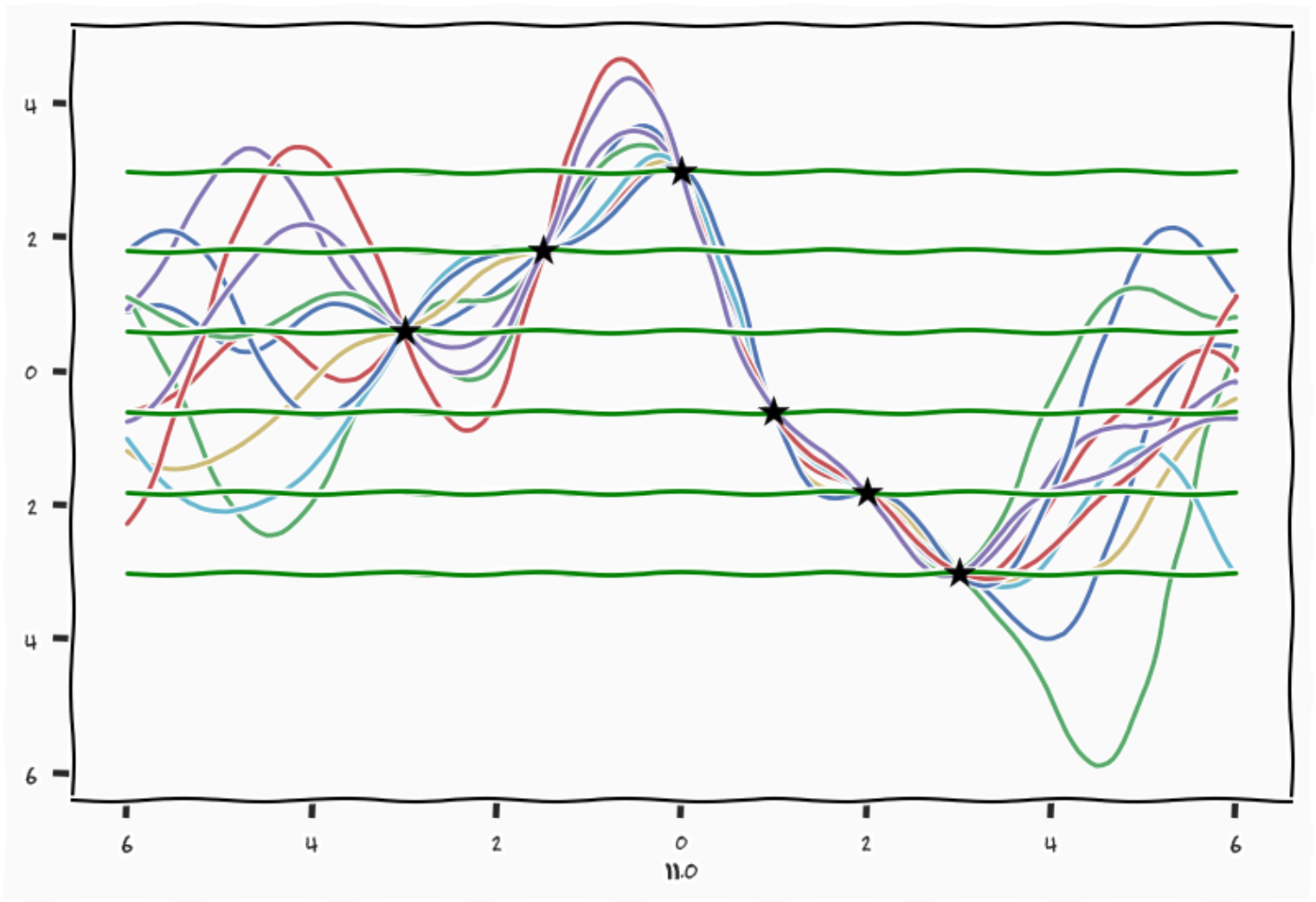


Gaussian Process Latent Variable Model [4]



[4] Lawrence, 2005

Gaussian Process Latent Variable Model [4]



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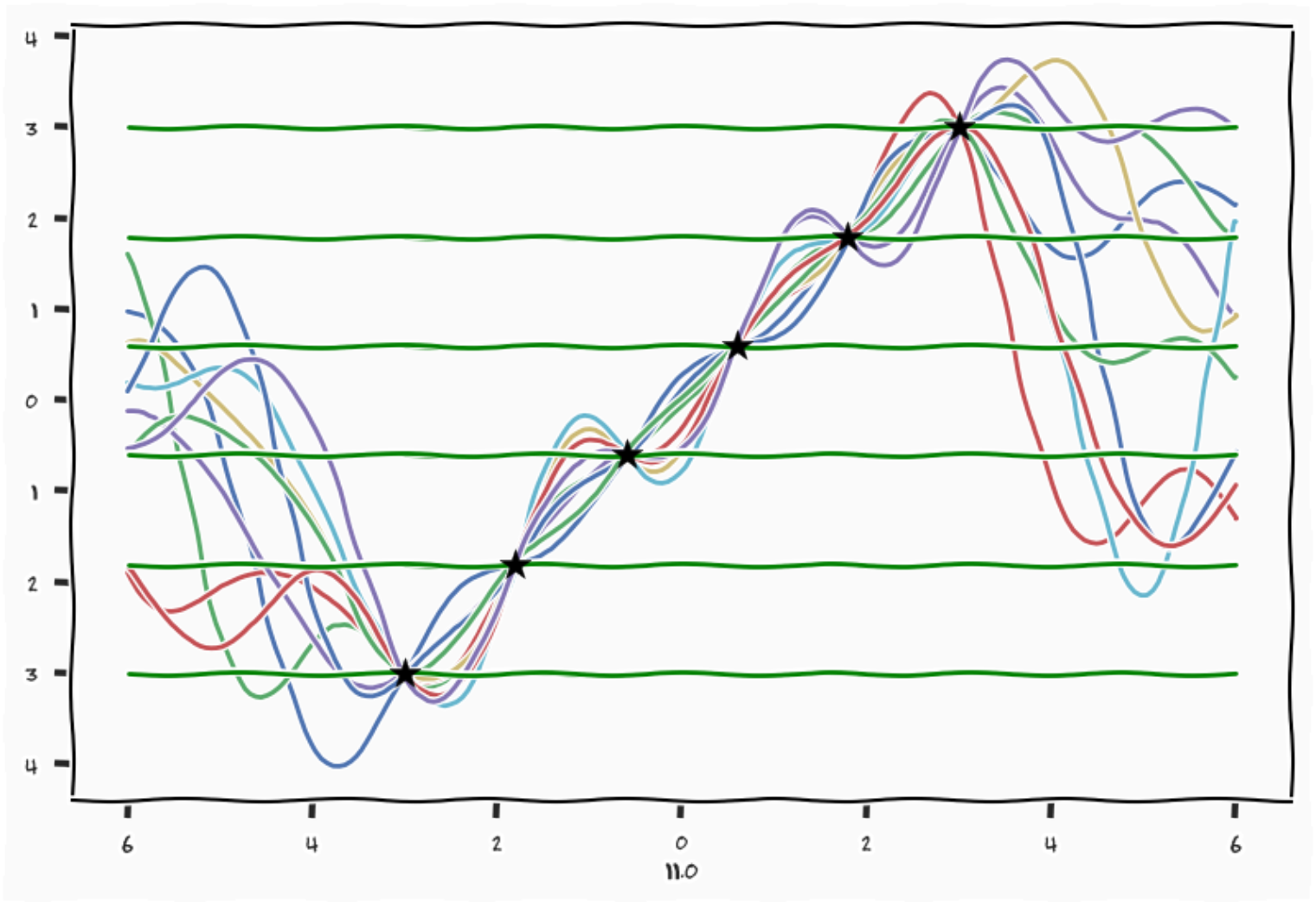
Gaussian Process Latent Variable Model [4]



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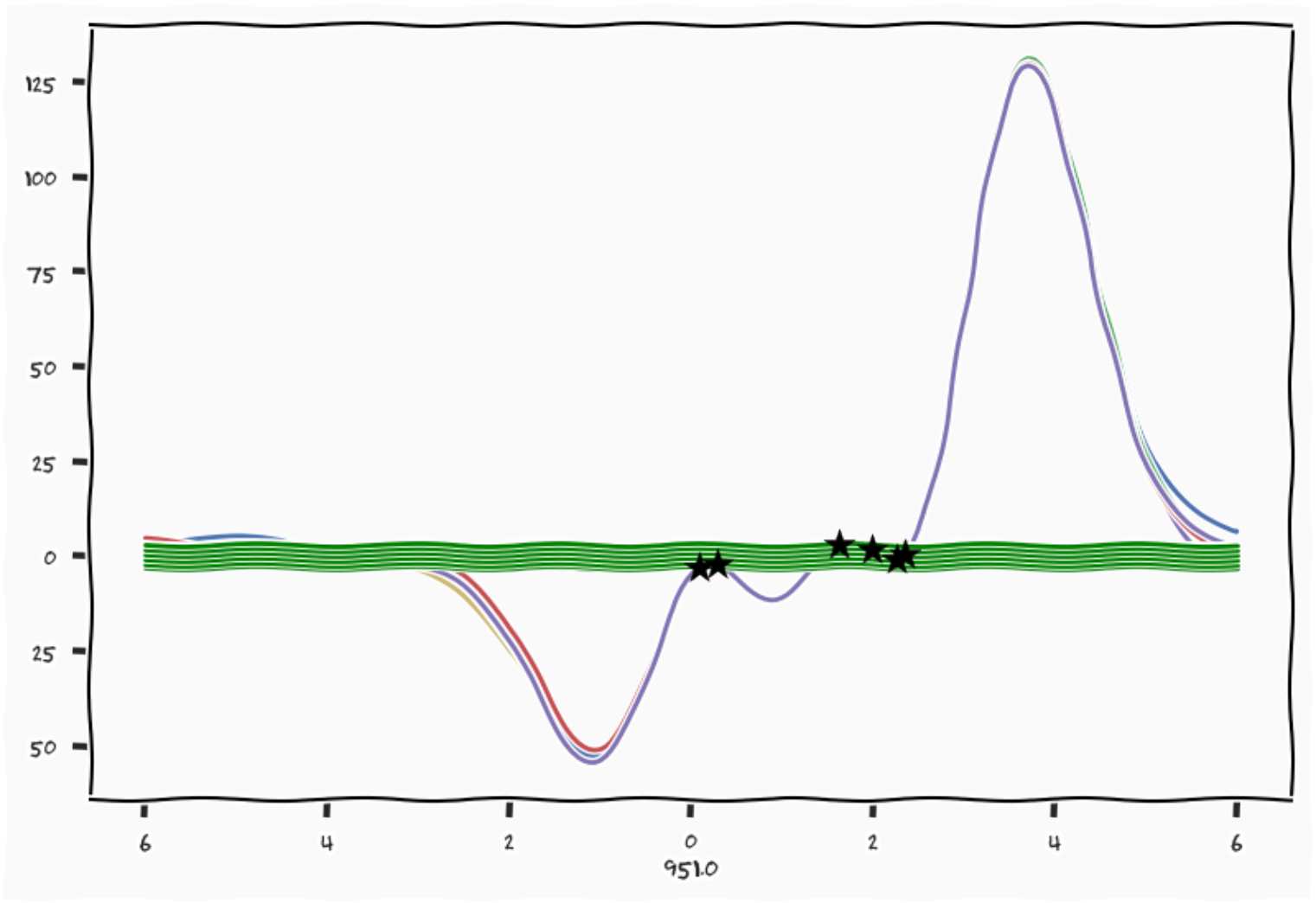
Gaussian Process Latent Variable Model [4]



[4] Lawrence, 2005

Priors

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

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. 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

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

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

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- Likelihood

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

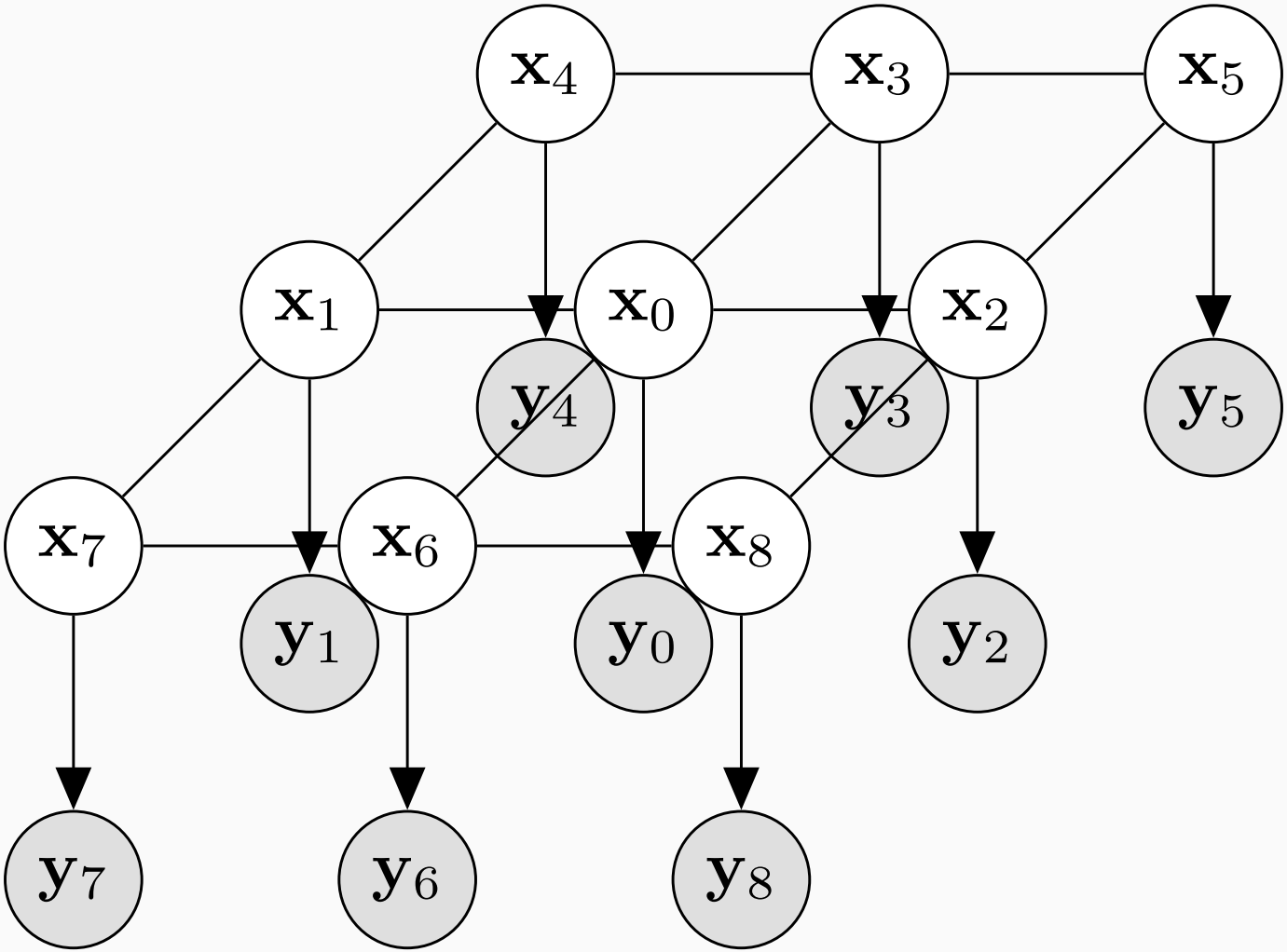
Laplace Integration

"Nature laughs at the difficulties of integrations"

– Simon Laplace

Image Segmentation

Markov Random Field



Markov Random Field

$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = \sum_{i}^{N} p(\mathbf{y}|\mathbf{x}_i)p(\mathbf{x}_i)$$

- $\mathbf{x}_i$ is a specific binary images

Numbers

- Possible black and white 3 Megapixel images

$$2^{3145728}$$

Numbers

- Possible black and white 3 Megapixel images

$$2^{3145728}$$

- Number of atoms in the universe

$$10^{80} \approx (2^{\frac{10}{3}})^{80} \approx 2^{267}$$

Numbers

- Possible black and white 3 Megapixel images

$$2^{3145728}$$

- Number of atoms in the universe

$$10^{80} \approx (2^{\frac{10}{3}})^{80} \approx 2^{267}$$

- Age of the universe in seconds

$$4.35 \cdot 10^{17} \approx 2^{59}$$

Intractability

- For most interesting problems computing the evidence is intractable
- Computational intractability: there are too many states to sum over
- Analytic: no closed form exists for the distribution

Today

- We have been living in a fairy land so far, the world is not conjugate

Today

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- We cannot give one lecture on approximate inference

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Today

- We have been living in a fairy land so far, the world is not conjugate
- We cannot give one lecture on approximate inference
- We hope to give you a flavour of approaches
    - Stochastic

Stochastic Inference

Basic Sampling

$$\mathbb{E}_{p(x)}[f] = \int f(x)p(x)\mathrm{d}x \approx \frac{1}{L}\sum_{l=1}^{L} f(x^{(l)}) = \hat{f}$$

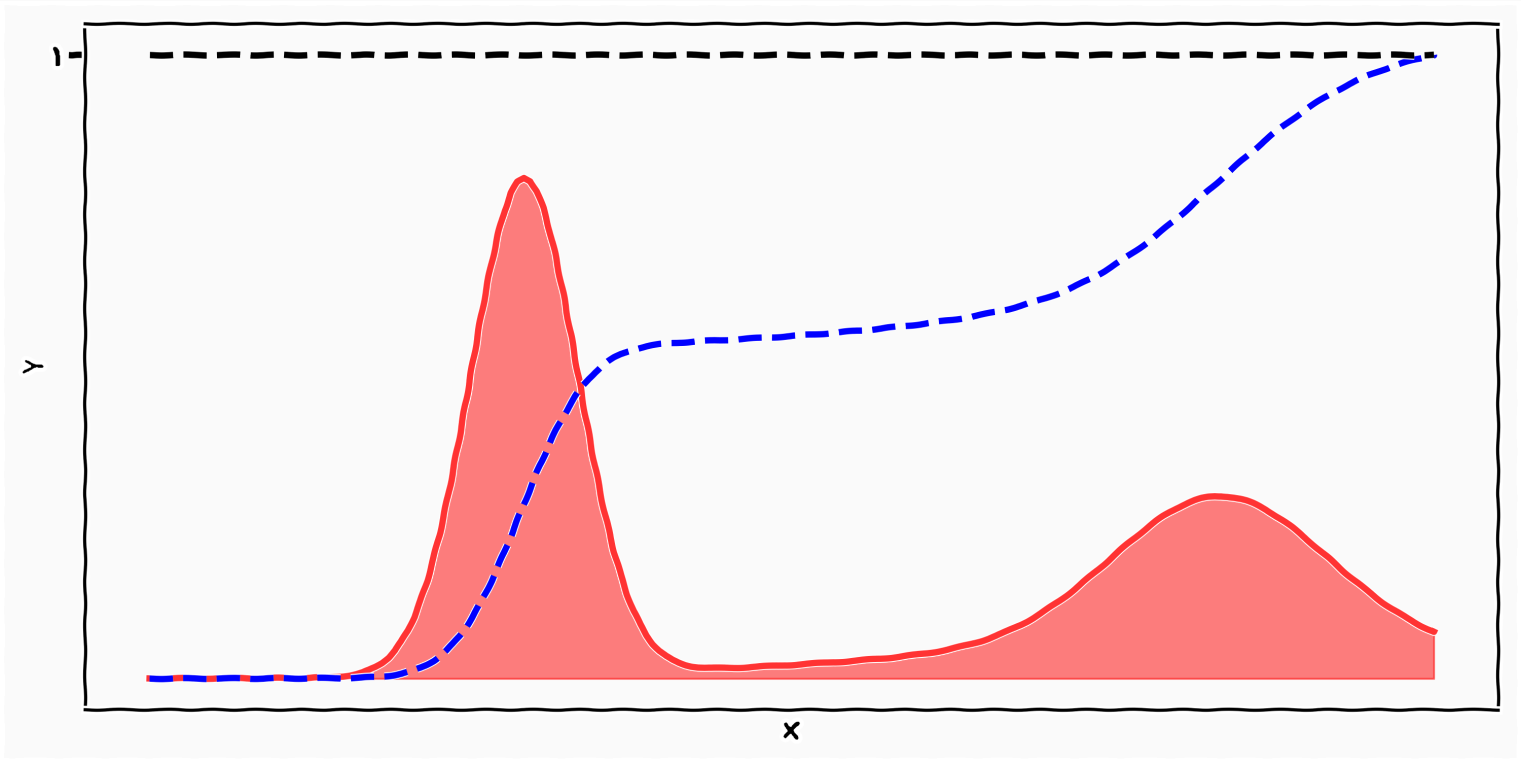
$$x^{(l)} \sim p(x)$$

$$\mathbb{E}[\hat{f}] = \mathbb{E}[f]$$

$$\mathsf{var}[\hat{f}] = \frac{1}{L}\mathbb{E}\left[(f(x) - \mathbb{E}[f])^2\right]$$

- Approximation not dependent on dimensionality of x
- Variance of estimator shrinks with number of samples

Basic Sampling

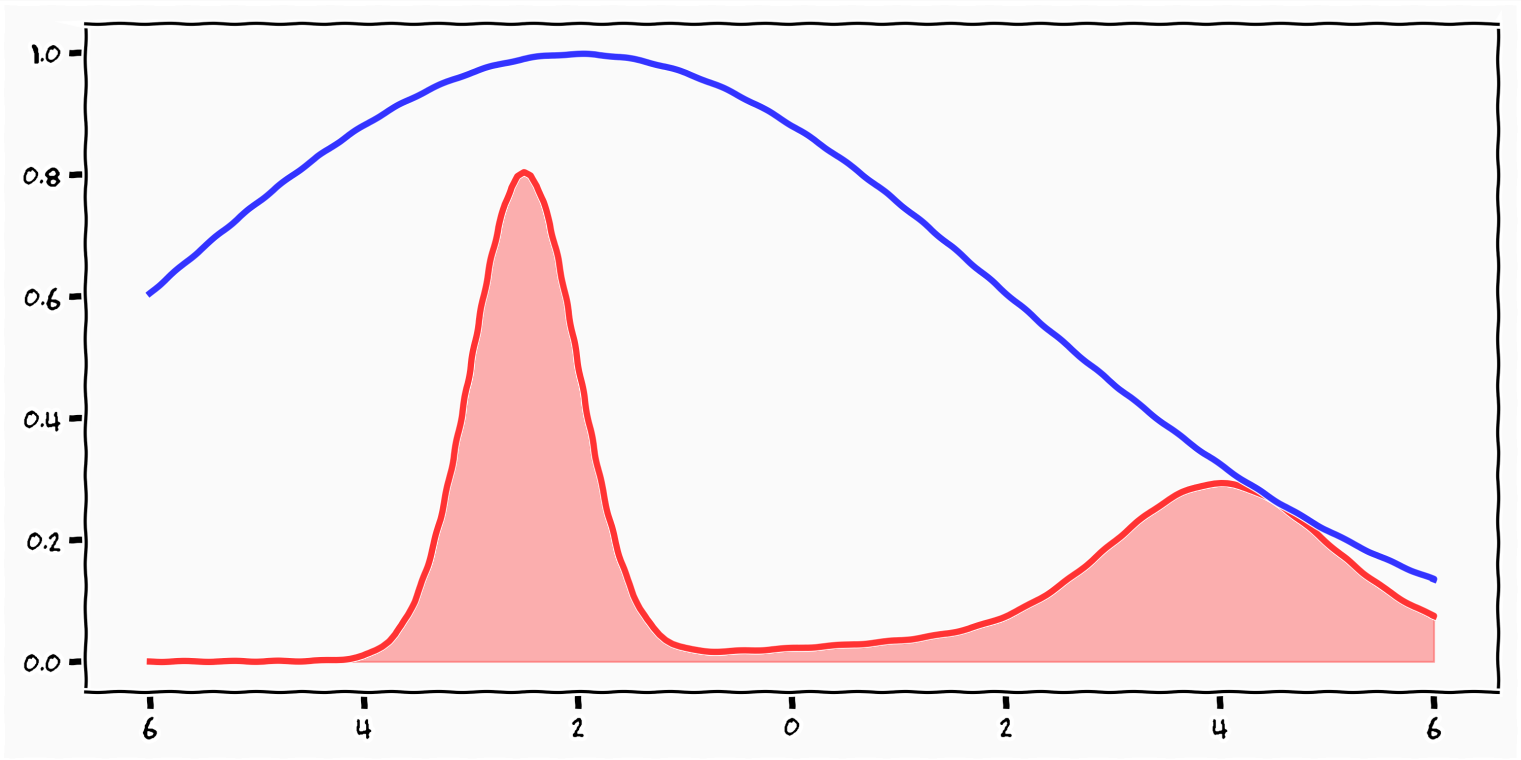


Sampling

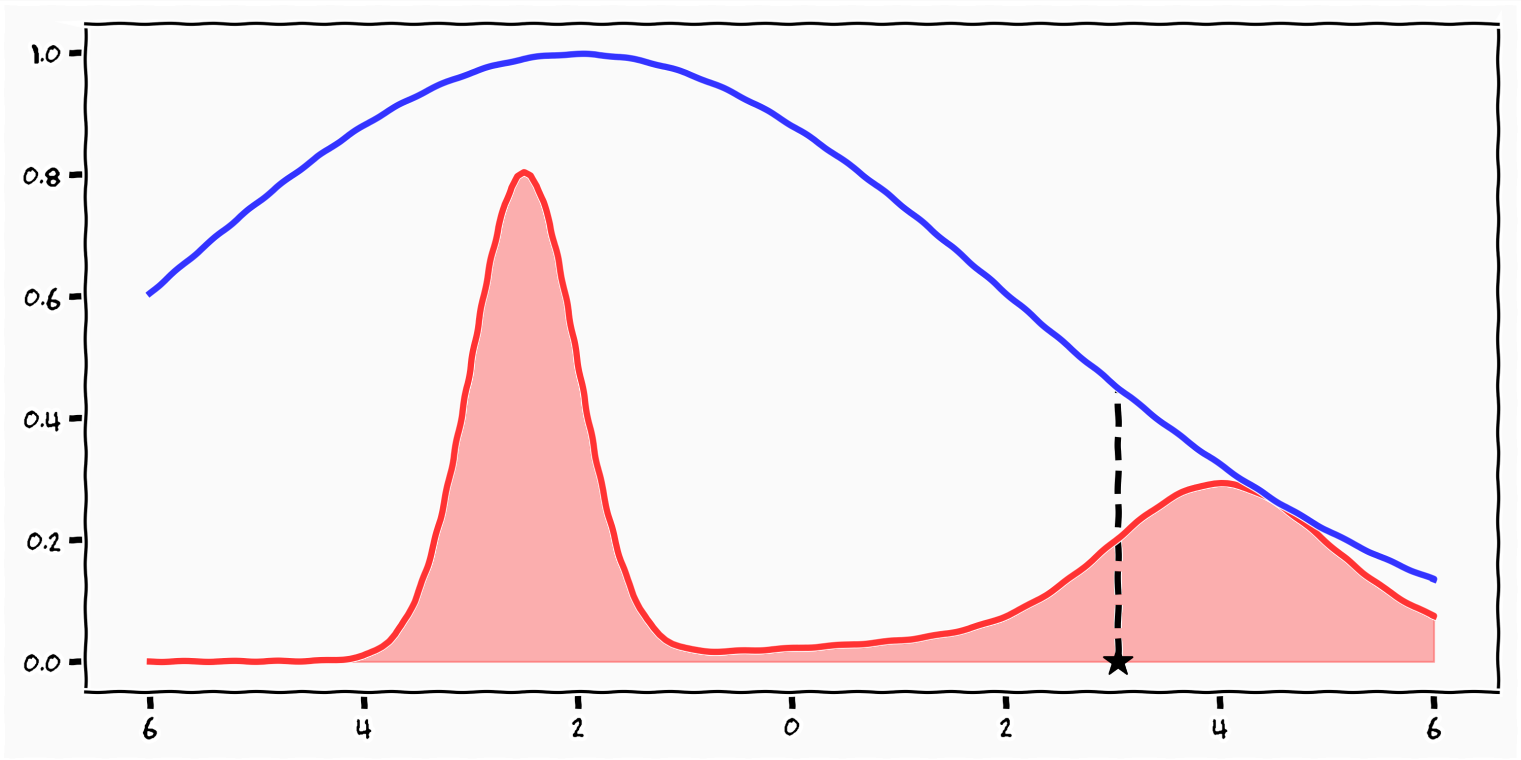
- We know how to transform samples from uniform to any distribution we can formulate the cummulative distribution
- Can we sample from distrubitons we do not know the form of?

    1. Rejection Sampling
    2. Importance Sampling

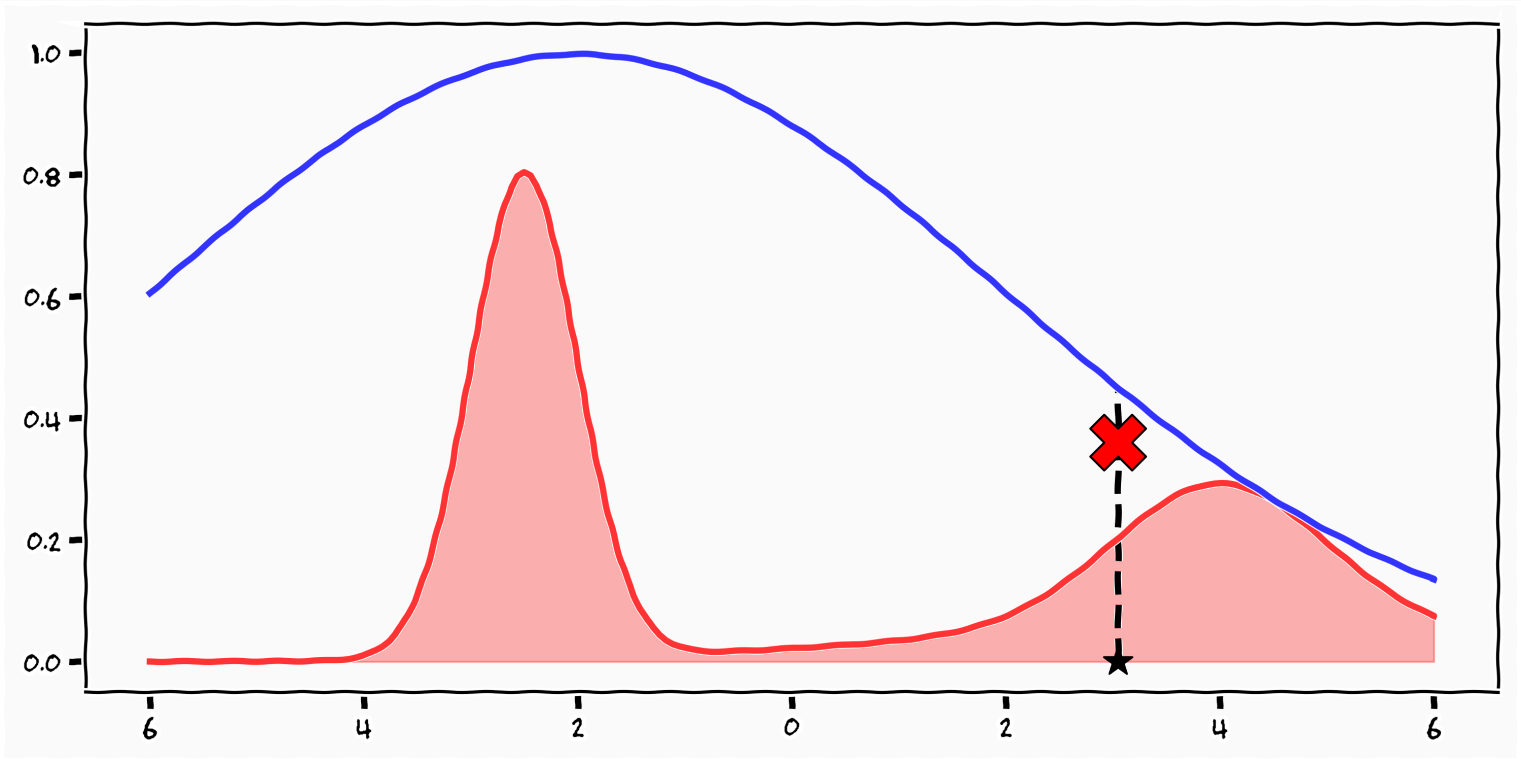
Rejection Sampling



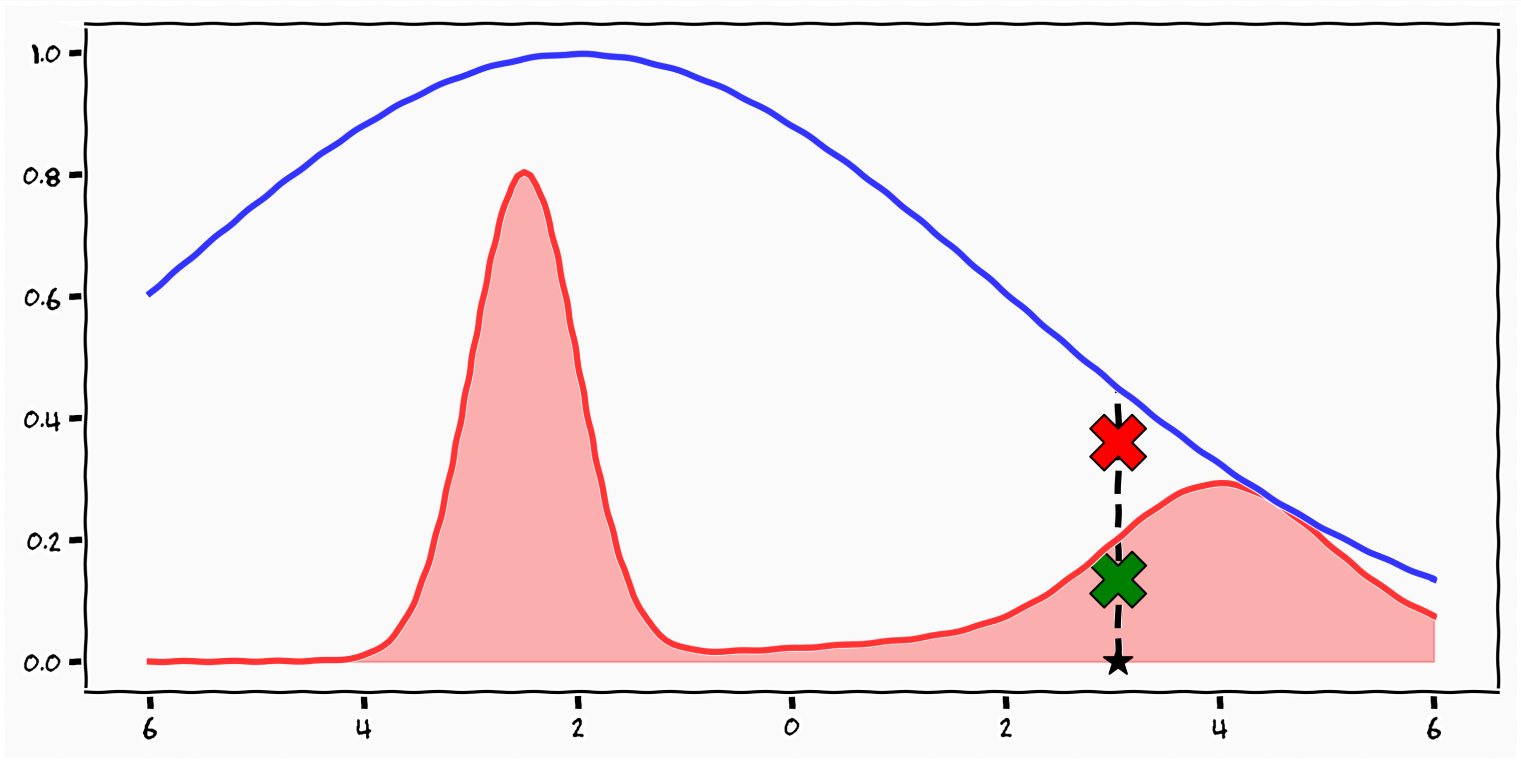
Rejection Sampling



Rejection Sampling



Rejection Sampling



Importance Sampling

$$\mathbb{E}_{p(x)}[f] = \int f(x)p(x)\mathrm{d}x$$

Importance Sampling

$$\mathbb{E}_{p(x)}[f] = \int f(x)p(x)\mathrm{d}x = \int f(x)p(x)\frac{q(x)}{q(x)}\mathrm{d}x$$

Importance Sampling

$$\begin{aligned}\mathbb{E}_{p(x)}[f] &= \int f(x)p(x)\mathrm{d}x = \int f(x)p(x)\frac{q(x)}{q(x)}\mathrm{d}x \\ &= \int f(x)\frac{p(x)}{q(x)}q(x)\mathrm{d}x\end{aligned}$$

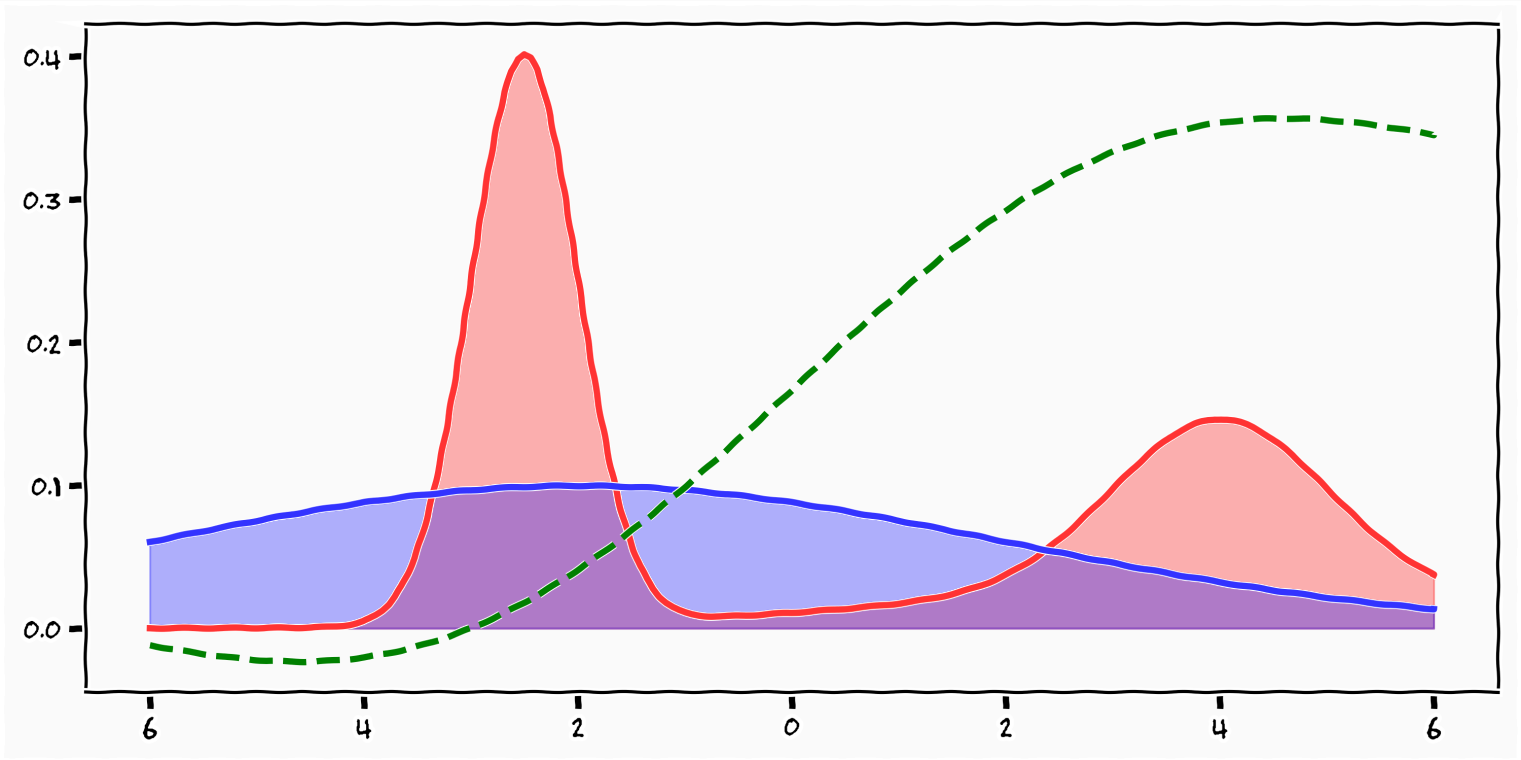
Importance Sampling

$$\begin{aligned}\mathbb{E}_{p(x)}[f] &= \int f(x)p(x)\mathrm{d}x = \int f(x)p(x)\frac{q(x)}{q(x)}\mathrm{d}x \\ &= \int f(x)\frac{p(x)}{q(x)}q(x)\mathrm{d}x = \mathbb{E}_{q(x)}\left[f(x)\frac{p(x)}{q(x)}\right]\end{aligned}$$

Importance Sampling

$$
\begin{aligned}
\mathbb{E}_{p(x)}[f] &= \int f(x)p(x)\mathrm{d}x = \int f(x)p(x)\frac{q(x)}{q(x)}\mathrm{d}x \\
&= \int f(x)\frac{p(x)}{q(x)}q(x)\mathrm{d}x = \mathbb{E}_{q(x)}\left[f(x)\frac{p(x)}{q(x)}\right] \\
&\approx \frac{1}{L}\sum_{l=1}^{L} f(x^{(l)})\frac{p(x^{(l)})}{q(x^{(l)})}
\end{aligned}
$$

Importance Sampling



Markov Chain Monte Carlo

- Sample from a proposal distribution
- Remembers the state and samples from a conditional
- Can lead to much better exploration of the space

Metropolis Sampling

1. start with state $x^{(0)}$

Metropolis Sampling

1. start with state $x^{(0)}$
2. sample from conditional proposal distribution $q(x^* \mid x^{(0)})$

Metropolis Sampling

1. start with state $x^{(0)}$
2. sample from conditional proposal distribution $q(x^* \mid x^{(0)})$
3. compute acceptance probability

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   - otherwise reject x^* and start over

Gibbs Sampling

- Often 1D samples are easy to get
- Gibbs sampling exploits this to create a very simple Markov Chain
- Sample each variable in turn conditioned on the others and cycle through

Gibbs Sampling

1. Initialise $x^{(0)}$

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5. cycle through variables

Why is this easier?

Multivariate case

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

$$p(\mathbf{y}) = \sum_i p(\mathbf{y}|\mathbf{x}^{(i)}) p(\mathbf{x}^{(i)})$$

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1D case

$$p(x_i|\mathbf{x}_{\neg i}, \mathbf{y}) = \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x}_{\neg i}, \mathbf{y})}$$
$$p(\mathbf{x}_{\neg i}, \mathbf{y}) = \int p(\mathbf{x}, \mathbf{y}) \mathrm{d}x_i = \sum_{x_i \in [1,-1]} p(x_i, \mathbf{x}_{\neg i}, \mathbf{y})$$
$$= p(x_i = 1, \mathbf{x}_{\neg i}, \mathbf{y}) + p(x_i = -1, \mathbf{x}_{\neg i}, \mathbf{y})$$

Summary

- There are lots and lots of sampling methods

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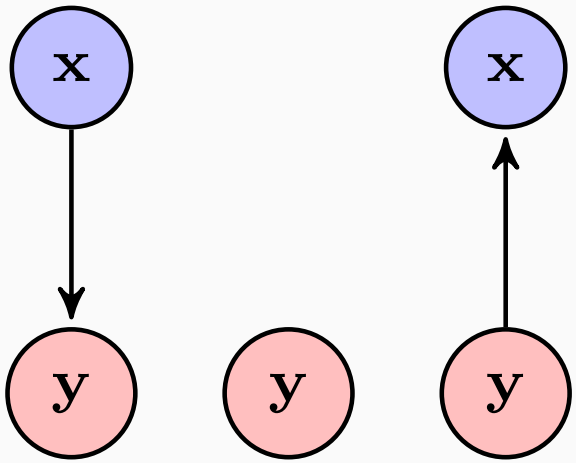
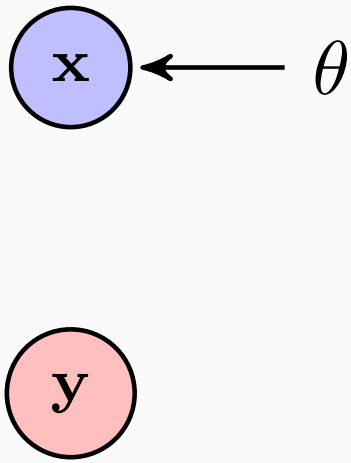
- Most provide quarantees in the limit
- Often requires a lot of problem knowledge to make efficient
- Hard to get a measure of how well you are doing

Deterministic Inference

Lower Bound





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

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Variational Bayes

$$p(y)$$

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Variational Bayes

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\begin{aligned}
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\end{aligned}
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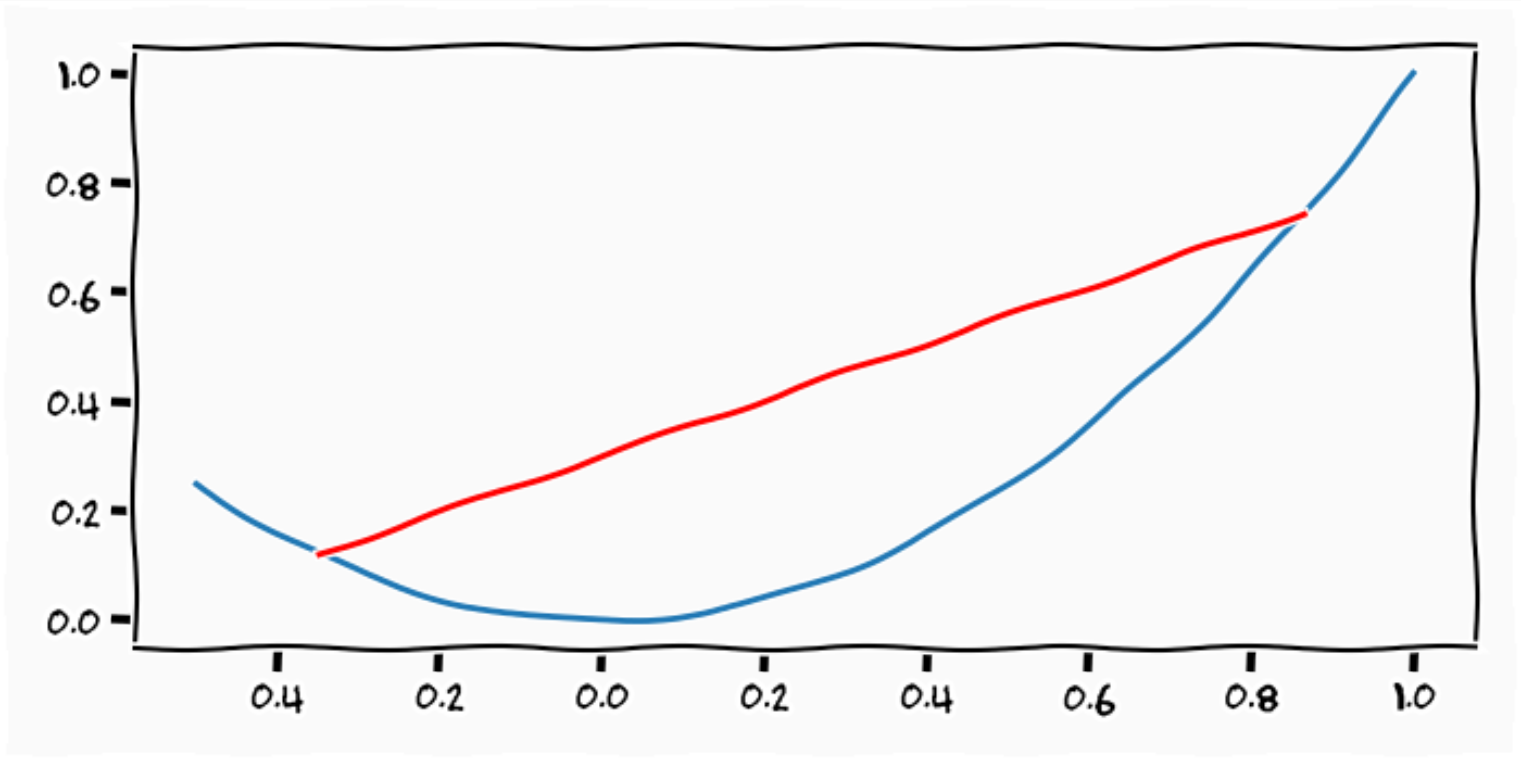
Jensen Inequality



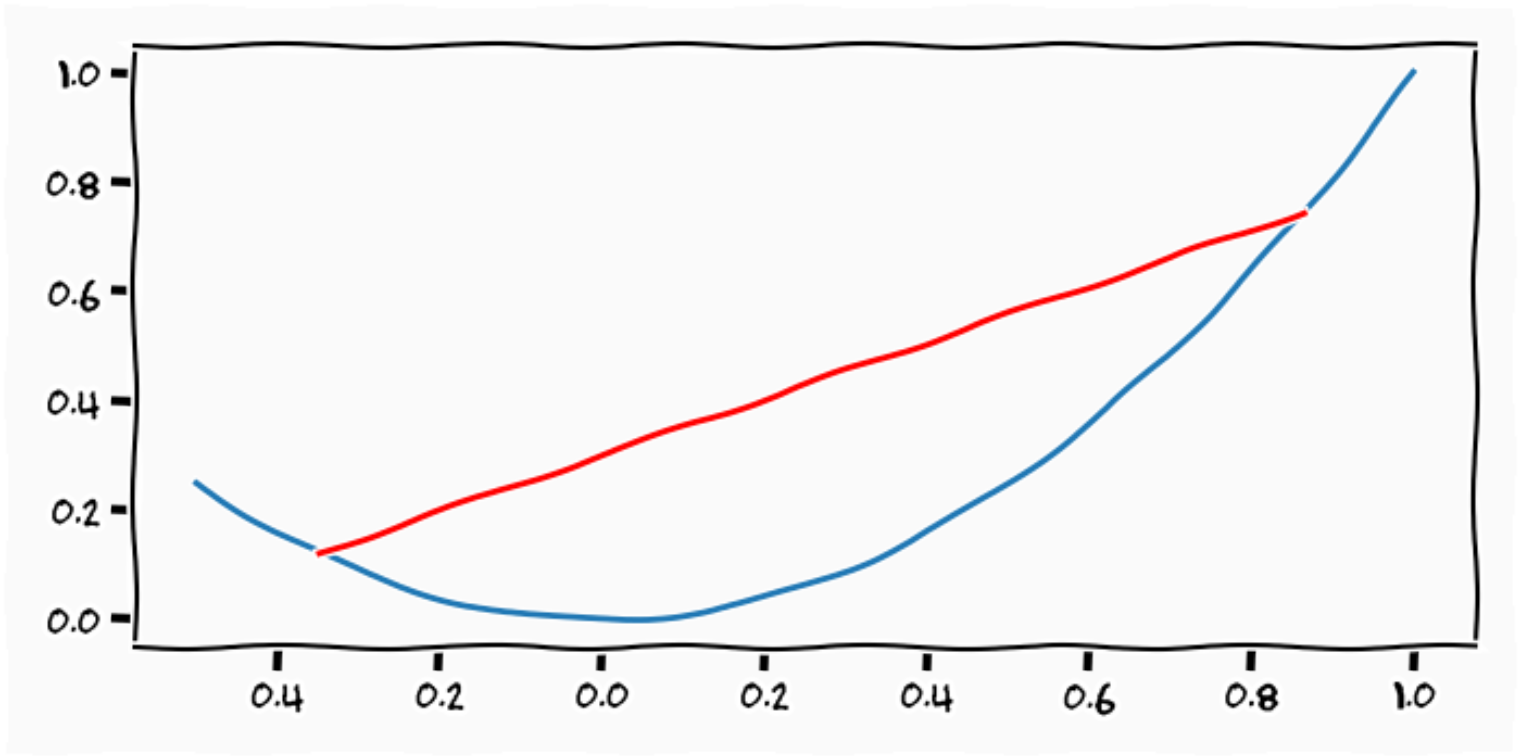
Convex Function

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

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

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

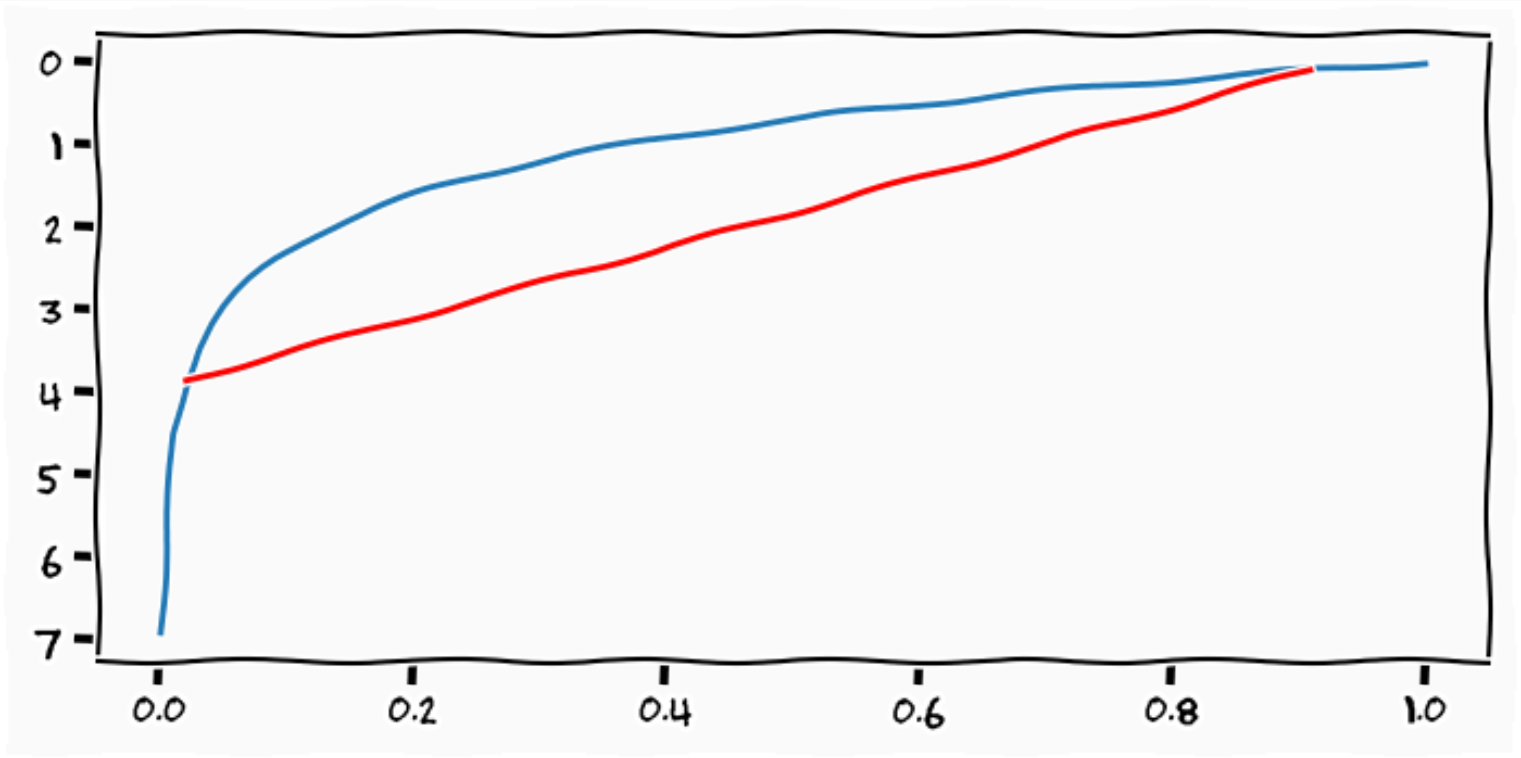
Jensen Inequality



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

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

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

The "posterior" term

$$\int q(x) \log \frac{q(x)}{p(x|y)} \mathrm{d}x$$

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$$\geq -\log \int p(x|y) \mathrm{d}x = -\log 1 = 0$$

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$$= 0$$

Kullback-Leibler Divergence

$$KL(q(x)||p(x|y)) = \int q(x) \log \frac{q(x)}{p(x|y)} \mathrm{d}x$$

- Measure of divergence between distributions
- Not a metric (not symmetric)
- $KL(q(x)||p(x|y)) = 0 \Leftrightarrow q(x) = p(x|y)$
- $KL(q(x)||p(x|y)) \geq 0$

The "other terms"

$$\int q(x)\log\frac{1}{q(x)}\mathrm{d}x + \int q(x)\log p(x,y)\mathrm{d}x =$$

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$$= \underbrace{\int p(x|y)\mathrm{d}x}_{=1}\log p(y) = \log p(y)$$

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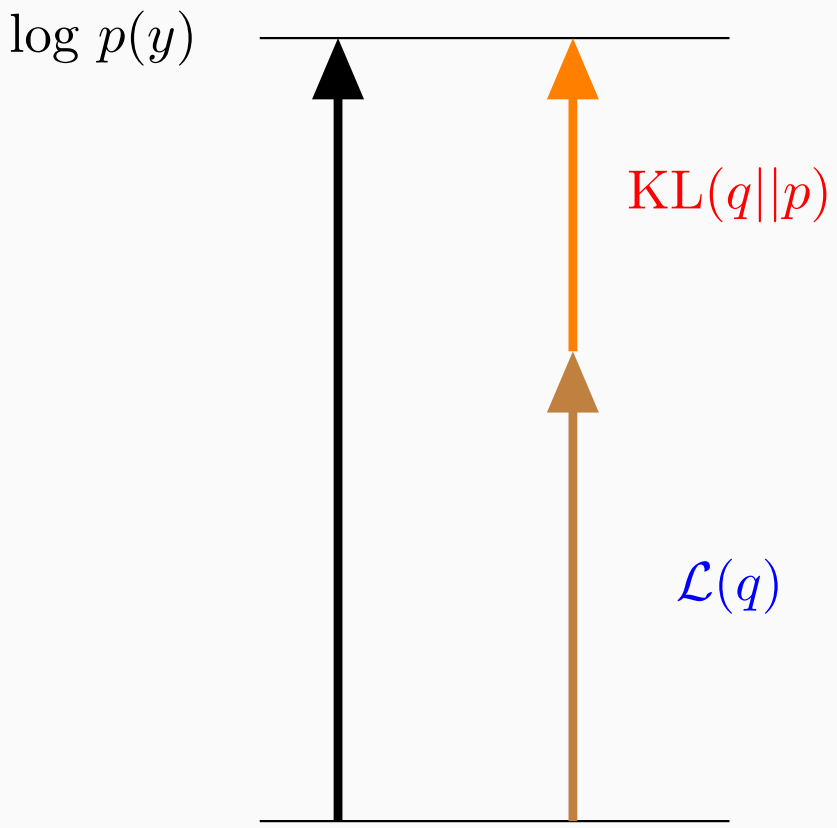
$$\log p(y) = \int q(x) \log \frac{1}{q(x)} \mathrm{d}x + \int q(x) \log p(x, y) \mathrm{d}x + \int q(x) \log \frac{q(x)}{p(x|y)} \mathrm{d}x$$

$$\geq - \int q(x) \log q(x) \mathrm{d}x + \int q(x) \log p(x, y) \mathrm{d}x$$

- The Evidence Lower BOnd
- Tight if $q(x) = p(x|y)$

Deterministic Approximation

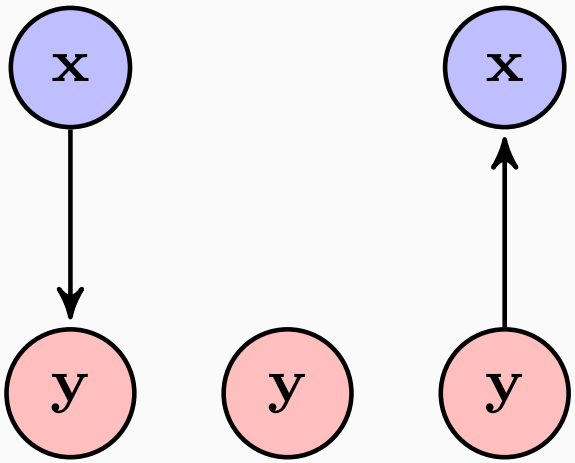


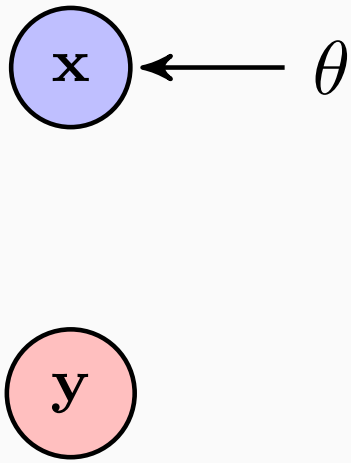
ELBO

$$\log p(y) \geq -\int q(x) \log q(x) \mathrm{d}x + \int q(x) \log p(x, y) \mathrm{d}x$$
$$= \mathbb{E}_{q(x)} \left[\log p(x, y) \right] - H(q(x)) = \mathcal{L}(q(x))$$

- if we maximise the ELBO we,
  - find an approximate posterior
  - lower bound the marginal likelihood
- *maximising* $p(y)$ is learning
- finding $q(x) \approx p(x|y)$ is prediction

Lower Bound





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Why is this a sensible thing to do?

– Ryan Adams[5]

[5] Talking Machines Podcast

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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[5]

[5] Talking Machines Podcast

How to choose Q?

$$\mathcal{L}(q(x)) = \mathbb{E}_{q(x)}\left[\log\, p(x, y)\right] - H(q(x))$$

- We have to be able to compute an expectation over the joint distribution
- The second term should be trivial

Mean Field Approximation

$$q(\mathbf{X}) = \prod_i q_i(\mathbf{x}_i)$$

$$\mathcal{L}(q_j) = \mathcal{L}_j(q_j) + \mathcal{L}_{\neg j}(q_{\neg j}),$$

- Model originating if Physics
- We model marginals rather than the full distribution
- We can update each distribution in turn and cycle

Summary

- Variational Bayes is never exact
- It can be made very fast
- There are exciting works using *implicit* variational distributions

Summary

Summary

- The evidence allows you to do model selection
  - "simple" is a relative concept that needs to be defined
- Most interesting things are intractable
- This leads to the field of approximative inference
  - you have gotten a "hint" of what is out there and some scaffolding to build upon

But what...

- *Now how about if we would treat the whole thing as a machine learning/inference problem instead?*

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- you can sample the integrand $\rightarrow$ data
- you kinda have an idea of the integral $\rightarrow$ prior
- you would be able to match the integral to data $\rightarrow$ likelihood
- and this we might talk about later in the course :-)

eof

References

Lawrence, Neil D (2005). "Probabilistic non-linear principal component analysis with Gaussian process latent variable models". In: *Journal of Machine Learning Research* 6, pp. 1783–1816.

Mean Field Approximation

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

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$$= \int \prod_i q_i(\mathbf{x}_i) \left(\log p(\mathbf{Y}, \mathbf{X}) - \sum_k \log q_k(\mathbf{x}_k) \right)$$

Mean Field Approximation

$$\mathcal{L}(q_j) = \int \prod_i q_i(\mathbf{x}_i) \left(\log p(\mathbf{Y}, \mathbf{X}) - \sum_k \log q_k(\mathbf{x}_k) \right) \mathrm{d}\mathbf{x}$$

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$$- \int_j q_j(\mathbf{x}_j) \int_{\neg j} \prod_{i \neq j} q(\mathbf{x}_i) \left(\log\, q_j(\mathbf{x}_j) + \sum_{k \neq j} \log\, q_k(\mathbf{x}_k) \right) \mathrm{d}\mathbf{x}_{\neg j} \mathrm{d}\mathbf{x}_j$$

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$$- \int_j q_j(\mathbf{x}_j) \int_{\neg j} \prod_{i \neq j} q(\mathbf{x}_i) \left(\log\, q_j(\mathbf{x}_j) + \sum_{k \neq j} \log\, q_k(\mathbf{x}_k) \right) \mathrm{d}\mathbf{x}_{\neg j} \mathrm{d}\mathbf{x}_j$$

Mean Field Approximation

$$= \int_j q_j(\mathbf{x}_j) \underbrace{\int_{\neg j} \prod_{i \neq j} q(\mathbf{x}_i) \log\, p(\mathbf{Y}, \mathbf{X}) \mathrm{d}\mathbf{x}_{\neg j}}_{\log\, f_j(\mathbf{x}_j)} \mathrm{d}\mathbf{x}_j$$

$$- \int_j q_j(\mathbf{x}_j) \int_{\neg j} \prod_{i \neq j} q(\mathbf{x}_i) \left(\log\, q_j(\mathbf{x}_j) + \sum_{k \neq j} \log\, q_k(\mathbf{x}_k) \right) \mathrm{d}\mathbf{x}_{\neg j} \mathrm{d}\mathbf{x}_j$$

$$= \int_j q_j(\mathbf{x}_j) \log\, f_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j$$

$$- \int_j q_j(\mathbf{x}_j) \left(\log\, q_j(\mathbf{x}_j) \underbrace{\int_{\neg j} \prod_{i \neq j} q_i(\mathbf{x}_i) \mathrm{d}\mathbf{x}_{\neg j}}_{=1} + \underbrace{\int_{\neg j} \prod_{i \neq j} q_i(\mathbf{x}_i) \sum_{k \neq j} \log\, q_k(\mathbf{x}_k) \mathrm{d}\mathbf{x}_{\neg j}}_{\text{constant w.r.t. } q_j} \right)$$

Mean Field Approximation

$$= \int_j q_j(\mathbf{x}_j) \log f_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j$$

$$- \int_j q_j(\mathbf{x}_j) \left(\log q_j(\mathbf{x}_j) \underbrace{\int_{\neg j} \prod_{i \neq j} q_i(\mathbf{x}_i) \mathrm{d}\mathbf{x}_{\neg j}}_{=1} + \underbrace{\int_{\neg j} \prod_{i \neq j} q_i(\mathbf{x}_i) \sum_{k \neq j} \log q_k(\mathbf{x}_k) \mathrm{d}\mathbf{x}_{\neg j}}_{\text{constant w.r.t. } q_j} \right) \mathrm{d}x_j$$

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$$= \int_j q_j(\mathbf{x}_j) \log f_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j - \int_j q_j(\mathbf{x}_j) \log q_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j + \text{const.} \cdot \underbrace{\int_j q_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j}_{=1}$$

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$$= \int_j q_j(\mathbf{x}_j) \log \frac{f_j(\mathbf{x}_j)}{q_j(\mathbf{x}_j)} \mathrm{d}\mathbf{x}_j + \text{const.}$$

Mean Field Approximation

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$$= \int_j q_j(\mathbf{x}_j) \log \frac{f_j(\mathbf{x}_j)}{q_j(\mathbf{x}_j)} \mathrm{d}\mathbf{x}_j + \text{const.}$$

$$= -\int_j q_j(\mathbf{x}_j) \log \frac{q_j(\mathbf{x}_j)}{f_j(\mathbf{x}_j)} \mathrm{d}\mathbf{x}_j + \text{const.}$$

Mean Field Approximation

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$$= -\int_j q_j(\mathbf{x}_j) \log \frac{q_j(\mathbf{x}_j)}{f_j(\mathbf{x}_j)} \mathrm{d}\mathbf{x}_j + \text{const.}$$

$$= -\mathrm{KL}(q_j(\mathbf{x}_j) || f_j(\mathbf{x}_j)) + \text{const.}$$

Mean Field Approximation

$$= \int_j q_j(\mathbf{x}_j) \log f_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j - \int_j q_j(\mathbf{x}_j) \log q_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j + \text{const.} \cdot \underbrace{\int_j q_j(\mathbf{x}_j) \mathrm{d}\mathbf{x}_j}_{=1}$$

$$= \int_j q_j(\mathbf{x}_j) \log \frac{f_j(\mathbf{x}_j)}{q_j(\mathbf{x}_j)} \mathrm{d}\mathbf{x}_j + \text{const.}$$

$$= -\int_j q_j(\mathbf{x}_j) \log \frac{q_j(\mathbf{x}_j)}{f_j(\mathbf{x}_j)} \mathrm{d}\mathbf{x}_j + \text{const.}$$

$$= -\mathrm{KL}(q_j(\mathbf{x}_j) || f_j(\mathbf{x}_j)) + \text{const.} = \mathcal{L}(q_j)$$

Mean Field Approximation

$$\mathcal{L}(q_j) = -\mathsf{KL}(q_j(\mathbf{x}_j)||f_j(\mathbf{x}_j)) + \text{const.}$$

- Want to maximise lower bound
- Negative KL $\rightarrow$ minimise KL term
- *we are free to choose the form of the distribution*

Mean Field Approximation

$$\log q_j(\mathbf{x}_j) = \log f_j(\mathbf{x}_j) = \int_{\neg j} \underbrace{\prod_{i \neq j} q_i(\mathbf{x}_i)}_{q_{\neg j}(\mathbf{x}_{\neg j})} \log p(\mathbf{Y}, \mathbf{X}) \mathrm{d}\mathbf{x}_{\neg j}$$

$$= \mathbb{E}_{q_{\neg j}(\mathbf{x}_{\neg j})} \left[\log p(\mathbf{Y}, \mathbf{X})\right]$$

- Choose the marginal distribution that makes the bound tight
- Will not make the bound tight in general though

Mean Field Variational Bayes

1. Formulate joint distribution over data and latent parameters

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3. Fit marginal approximation by making bound tight
4. Iterate through variables

Taking stock

- We have derived a general update for the mean-field approximation

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- We have derived a general update for the mean-field approximation
- Looks an awful lot like Expectation-Maximisation
  - EM is VB (E-local, M-global)
- Looks an awful lot like Gibbs sampling
  - Gibbs: sample from complete conditional
  - VB: variational expectations of natural parameters of the complete conditional