Gaussian processes for non-Gaussian likelihoods

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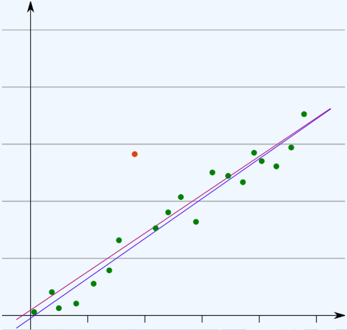
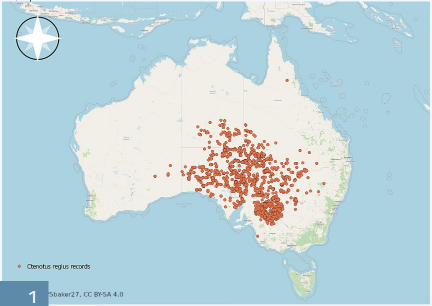
Finnish Center for Artificial Intelligence
& Aalto University

Gaussian Process Summer School, 14 September 2021

Not Gaussian noise





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Overview

Outline:

1. **Gaussian processes with Gaussian likelihood**
2. What is the likelihood? Connecting observations and Gaussian process prior
3. Non-Gaussian likelihoods: what happens to the posterior?
4. How to approximate the intractable
5. Comparisons

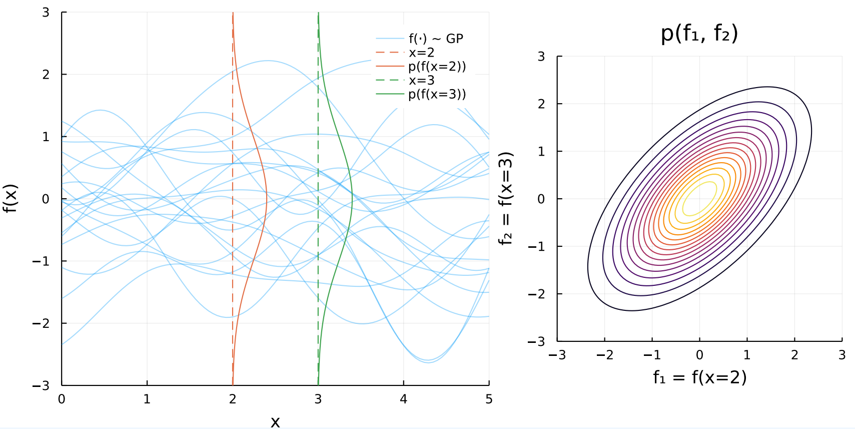
+ *Intuitive* understanding
+ Learning the language

– In-depth expertise
– Lots of maths

Setting the scene

Gaussian process $f(\cdot)$

Distribution over *functions*
Marginals are Gaussian (mean and covariance)

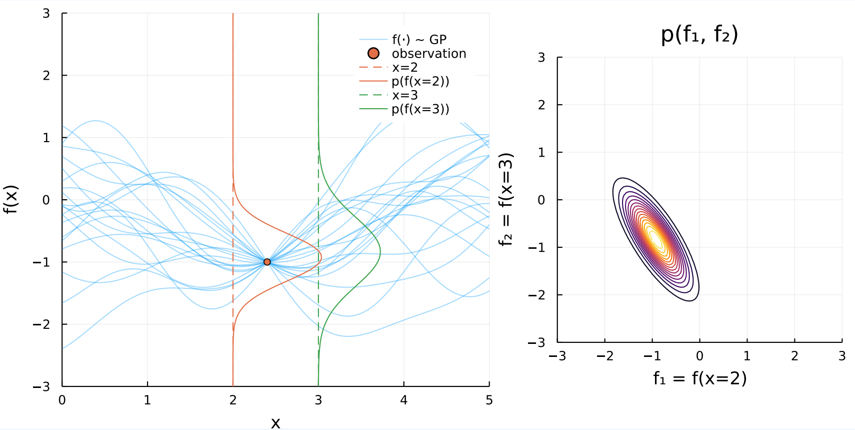


infinitecuriosity.org/vizgp

Gaussian process conditioned on observation

Distribution over *functions*

Marginals are Gaussian (mean and covariance)

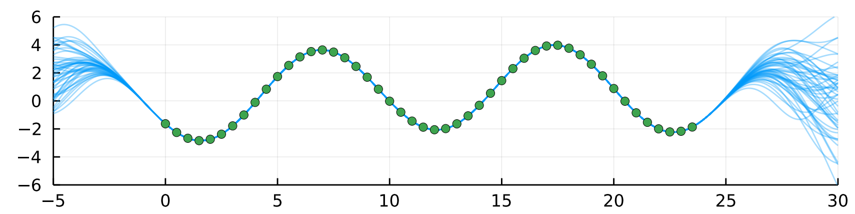


infinitecuriosity.org/vizgp

Gaussian noise model

$$y(x) = f(x) + \epsilon, \qquad \epsilon \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2_{\text{noise}})$$

$$p(y \mid f) = \mathcal{N}(y \mid f, \sigma^2_{\text{noise}})$$



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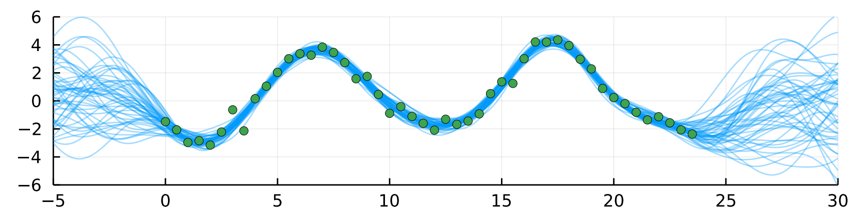
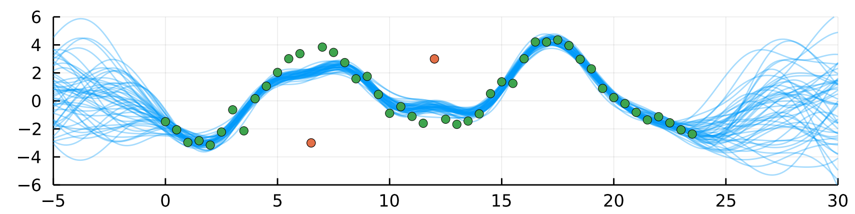


Misspecified Gaussian noise model

$$y(x) = f(x) + \epsilon, \qquad \epsilon \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2_{\text{noise}})$$

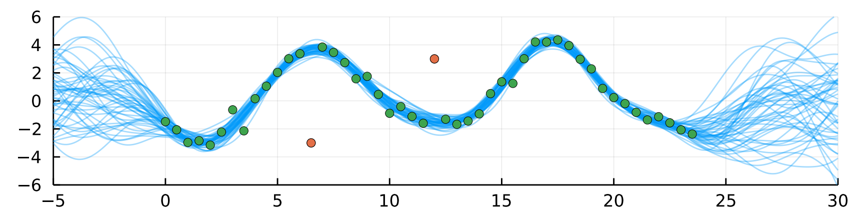
$$p(y \,|\, f) = \mathcal{N}(y \,|\, f, \sigma^2_{\text{noise}})$$



HEAVY-TAILED NOISE MODEL

$$y(x) = f(x) + \epsilon, \qquad \epsilon \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2_{\text{noise}})$$

$$p(y \mid f) = \mathcal{N}(y \mid f, \sigma^2_{\text{noise}})$$



Outline

✓ Gaussian processes with Gaussian likelihood

2. **What is the likelihood? Connecting observations and Gaussian process prior**
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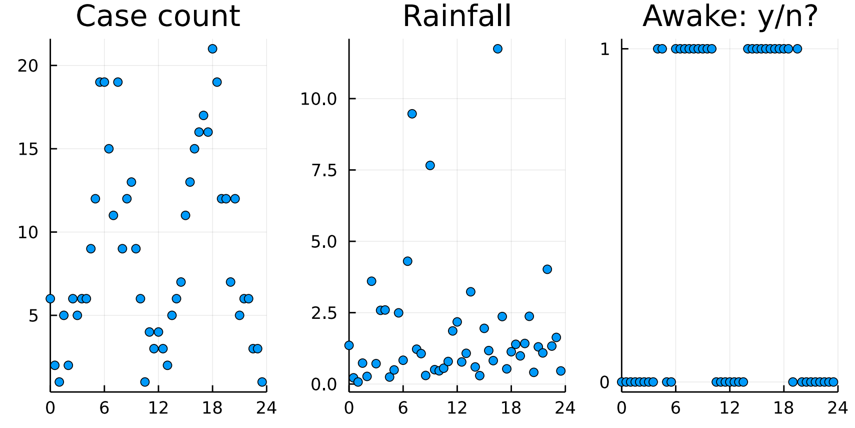
Likelihood

Non-Gaussian observations



latent functional relationship

Likelihood

$$p(\mathbf{y}\,|\,\mathbf{f}) = \prod_{i=1}^{N} p(y_i\,|\,f_i); \qquad f_i = f(x_i)$$

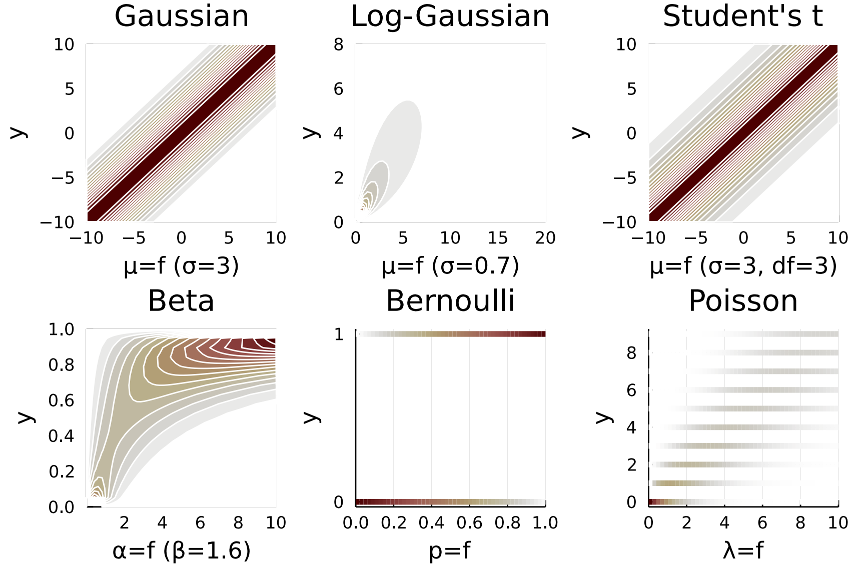
factorizing

$$p(y\,|\,f)$$

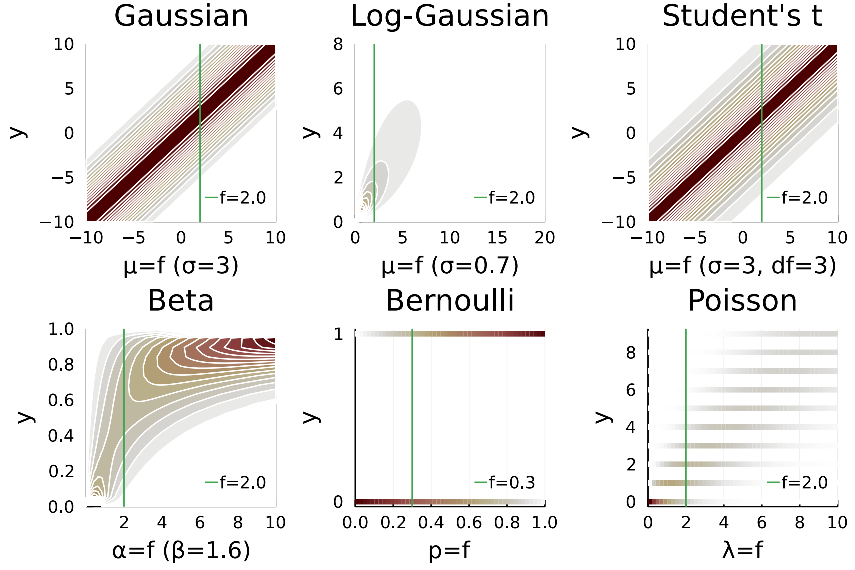
Function of two arguments:

$$y \mapsto p(y\,|\,f), \qquad f \mapsto p(y\,|\,f)$$

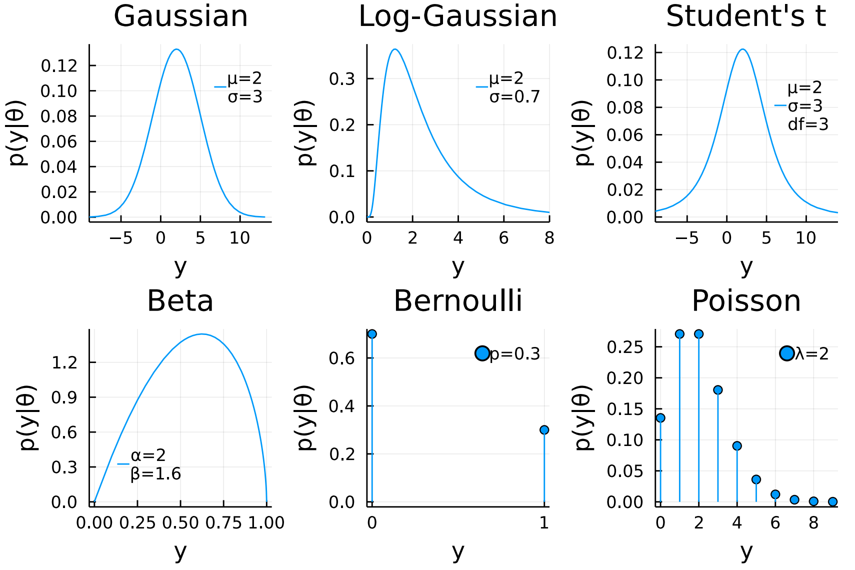
$p(y\mid f)$


Gaussian
y
10
5
0
−5
−10
−10
−5
0
5
10
μ=f (σ=3)
Log-Gaussian
y
8
6
4
2
0
0
5
10
15
20
μ=f (σ=0.7)
Student's t
y
10
5
0
−5
−10
−10
−5
0
5
10
μ=f (σ=3, df=3)
Beta
y
1.0
0.8
0.6
0.4
0.2
0.0
2
4
6
8
10
α=f (β=1.6)
Bernoulli
y
1
0
0.0
0.2
0.4
0.6
0.8
1.0
p=f
Poisson
y
8
6
4
2
0
0
2
4
6
8
10
λ=f

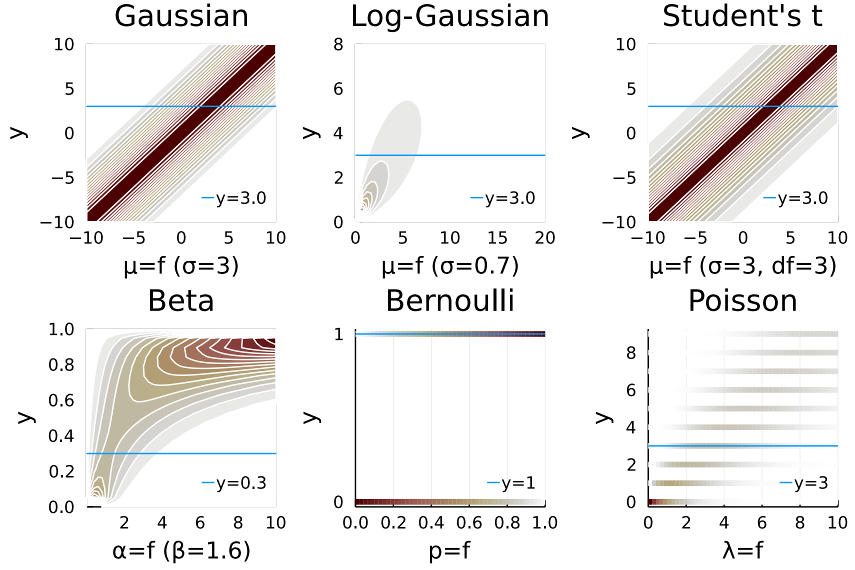
$p(y \mid f)$: DISTRIBUTION OF OBSERVATION f FIXED



$p(y \mid f)$: DISTRIBUTION OF OBSERVATION $\quad f$ FIXED



$p(y \mid f)$: LIKELIHOOD OF PARAMETER y FIXED



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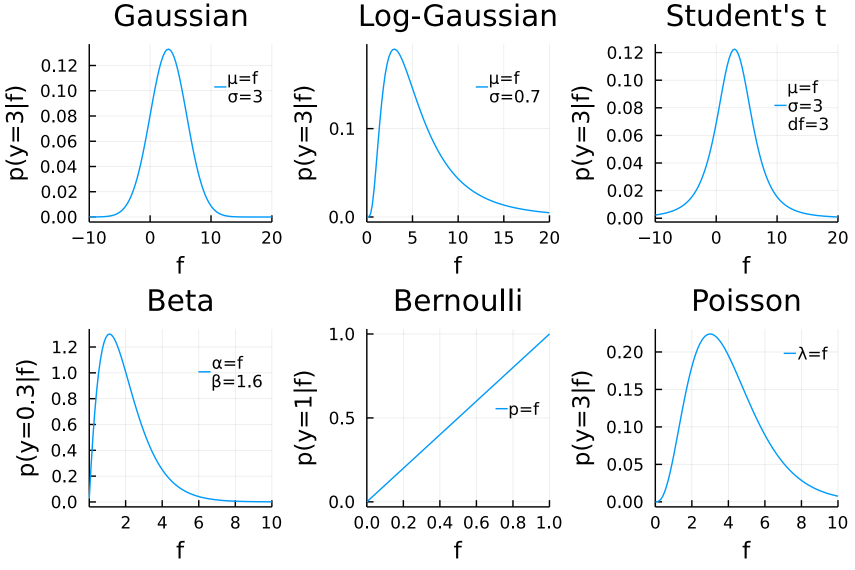


$p(y \mid f)$: LIKELIHOOD OF PARAMETER y FIXED

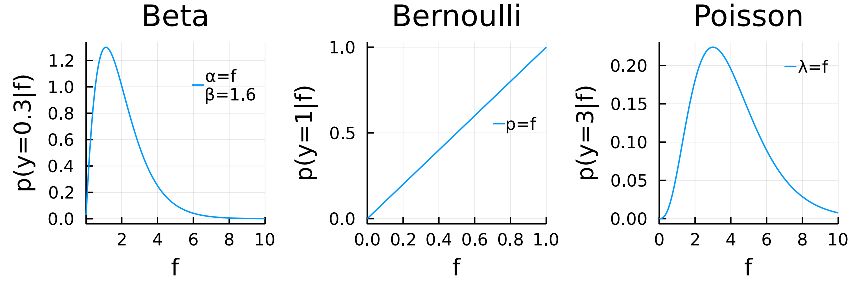
Two aspects of likelihoods:

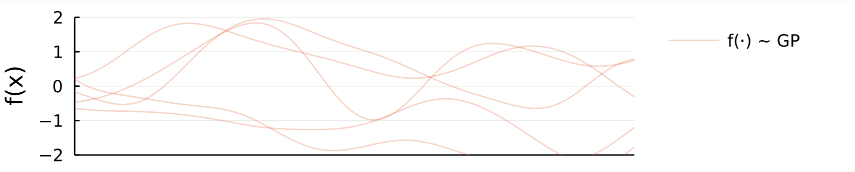
1. link functions
2. log-concavity

Link functions

$$\mathbb{E}[y] = \theta \in (0 \ldots \infty) \qquad \mathrm{link}(\theta) = f$$

$$f \sim \mathcal{N} \qquad \in (-\infty \ldots \infty) \qquad \theta = \mathrm{invlink}(f)$$





Link functions

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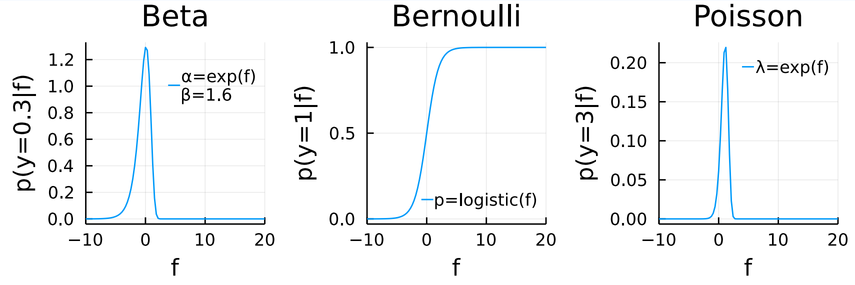

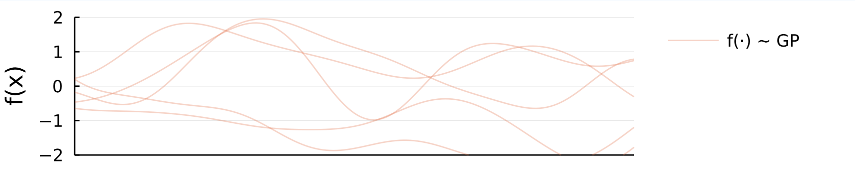

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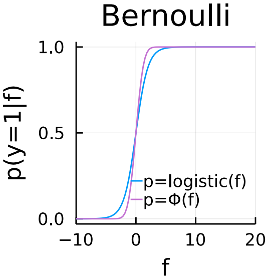
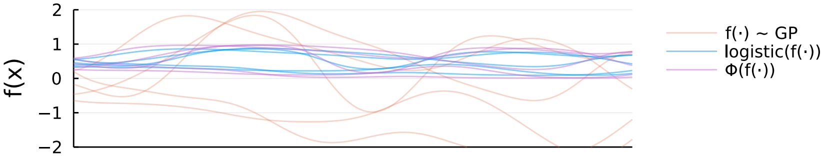
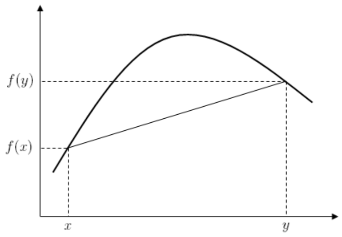


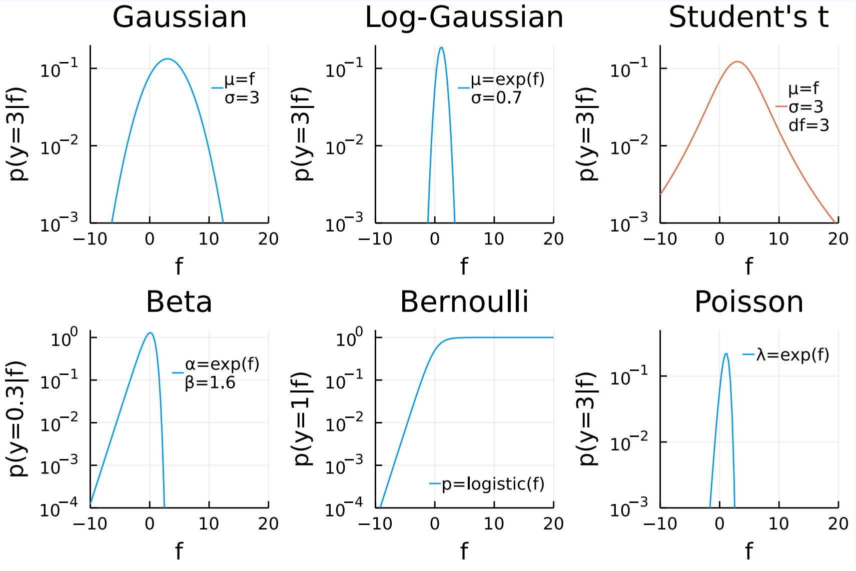


(Log-)concavity



$$f\left(\alpha x + (1-\alpha)y\right) \geq \alpha f(x) + (1-\alpha)f(y)$$

Log-concavity of likelihoods



Outline

✓ Gaussian processes with Gaussian likelihood

✓ What is the likelihood? Connecting observations and Gaussian process prior

3. **Non-Gaussian likelihoods: what happens to the posterior?**
4. How to approximate the intractable
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Posterior

Likelihood

$$p(y \mid f)$$

Joint distribution

$$p(y, f) = p(y \mid f)p(f)$$

Posterior

$$f \mapsto p(f \mid y) = \frac{p(y \mid f)p(f)}{p(y)}$$

$$y \mapsto \big(f \mapsto p(f \mid y)\big)$$

Posterior predictions

At new point x^*:

$$p(f^* \mid x^*, \mathbf{x}, \mathbf{y}) = \int p(f^* \mid x^*, \mathbf{x}, \mathbf{f})\, p(\mathbf{f} \mid \mathbf{x}, \mathbf{y})\, \mathrm{d}\mathbf{f}$$

At training data:

$$p(\mathbf{f} \mid \mathbf{x}, \mathbf{y}) = \frac{p(\mathbf{f} \mid \mathbf{x}) \prod_{i=1}^{N} p(y_i \mid f(x_i))}{\int p(\mathbf{f}' \mid \mathbf{x}) \prod_{i=1}^{N} p(y_i \mid f'(x_i))\, \mathrm{d}\mathbf{f}''}$$

$$p(\mathbf{f} \mid \mathbf{y}) = \frac{1}{Z} p(\mathbf{f}) \prod_{i=1}^{N} p(y_i \mid f_i)$$

$$Z = p(\mathbf{y} \mid \mathcal{M}) = \int p(\mathbf{f} \mid \mathcal{M}) \prod_{i=1}^{N} p(y_i \mid f_i, \mathcal{M})\, \mathrm{d}\mathbf{f}$$

“marginal likelihood” or “evidence” given model $\mathcal{M}$

Posterior

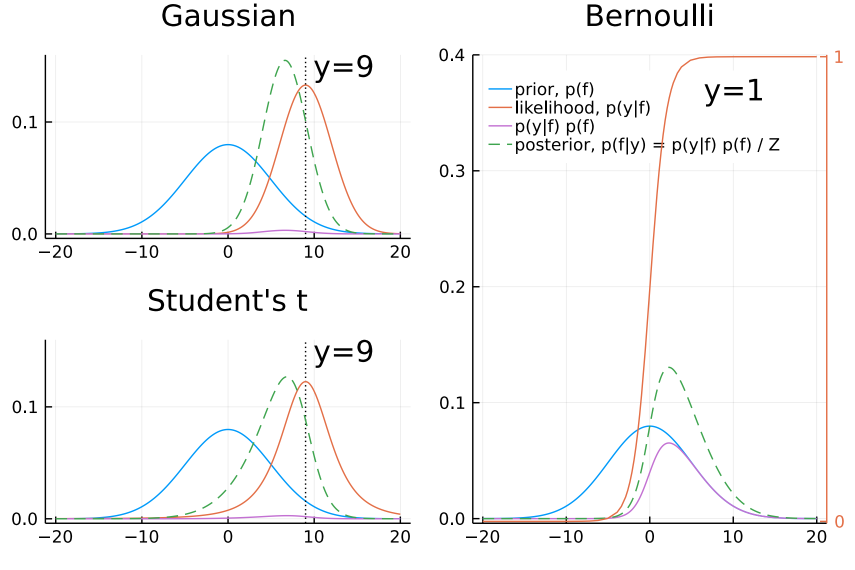
$$p(\mathbf{f} \mid \mathbf{y}) = \frac{1}{Z} p(\mathbf{f}) \prod_{i=1}^{N} p(y_i \mid f_i)$$

Gaussian (process) prior $p(f(\cdot))$ …

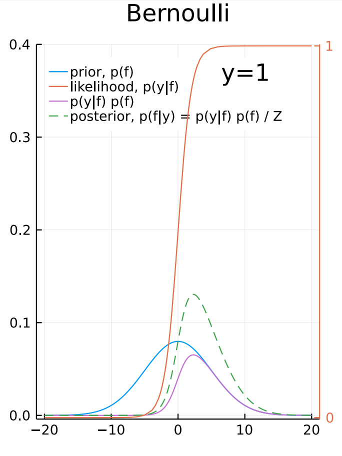
& Gaussian likelihood: conjugate case → posterior Gaussian

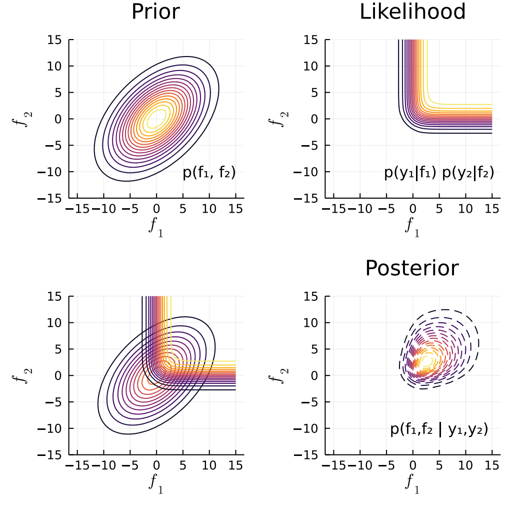
& non-Gaussian $p(y|f) \rightarrow p(\mathbf{f} \mid \mathbf{y})$ also non-Gaussian, intractable

1D EXAMPLES


Gaussian
y=9
0.1
0.0
−20
−10
0
10
20
Student's t
y=9
0.1
0.0
−20
−10
0
10
20
Bernoulli
y=1
prior, p(f)
likelihood, p(y|f)
p(y|f) p(f)
posterior, p(f|y) = p(y|f) p(f) / Z
0.4
0.3
0.2
0.1
0.0
1
0
−20
−10
0
10
20

Bernoulli example in 2D





Posterior for N observations

$$p(\mathbf{f} \mid \mathbf{y}) = \frac{p(\mathbf{f}) \prod_{i=1}^{N} p(y_i \mid f_i)}{\int p(\mathbf{f}') \prod_{i=1}^{N} p(y_i \mid f_i') \mathrm{d}\mathbf{f}'}$$

$$\begin{aligned} f_1 &= f(x_1) \\ f_2 &= f(x_2) \\ &\vdots \\ f_N &= f(x_N) \end{aligned}$$

Summary so far

- What is the likelihood $p(y \mid f)$?
- When is it non-Gaussian?
- Why does the posterior $p(f \mid y)$ become intractable?

Questions?! :)

Outline

✓ Gaussian processes with Gaussian likelihood

✓ What is the likelihood? Connecting observations and Gaussian process prior

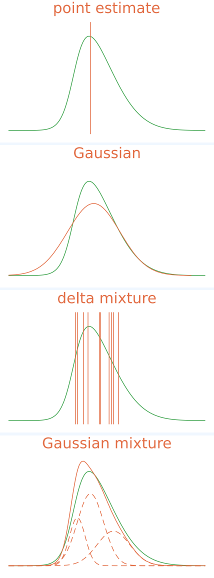
✓ Non-Gaussian likelihoods: what happens to the posterior?

4. **How to approximate the intractable**
5. Comparisons

Approximations

Approximating distributions

- delta distribution
  - point estimate
- **Gaussian distribution**
  - Laplace
  - Expectation Propagation (EP)
  - Variational Bayes/Variational Inference (VB / VI)
- mixture of delta distributions
  - Markov Chain Monte Carlo (MCMC)
- mixture of Gaussians
- …



Gaussian approximations

Approximating the exact posterior with Gaussian

Approximating the posterior at observations:

$$p(\mathbf{f} \mid \mathbf{y}) \approx q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mu =?, \Sigma =?)$$

Predictions at new points:

$$p(f^* \mid x^*, \mathbf{y}) \approx q(f^*) = \int p(f^* \mid x^*, \mathbf{f})\, q(\mathbf{f})\, \mathrm{d}\mathbf{f}$$

Demo: What does this mean for Gaussian processes?

Choosing μ and Σ for $q(\mathbf{f})$

$$p(\mathbf{f} \mid \mathbf{y}) \approx q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mu = ?, \Sigma = ?)$$

match mean & variance at point

minimise divergence

Laplace approximation

Expectation Propagation (EP)

Variational Bayes (VB)

Laplace approximation

Laplace approximation

Idea: log of Gaussian pdf = quadratic polynomial

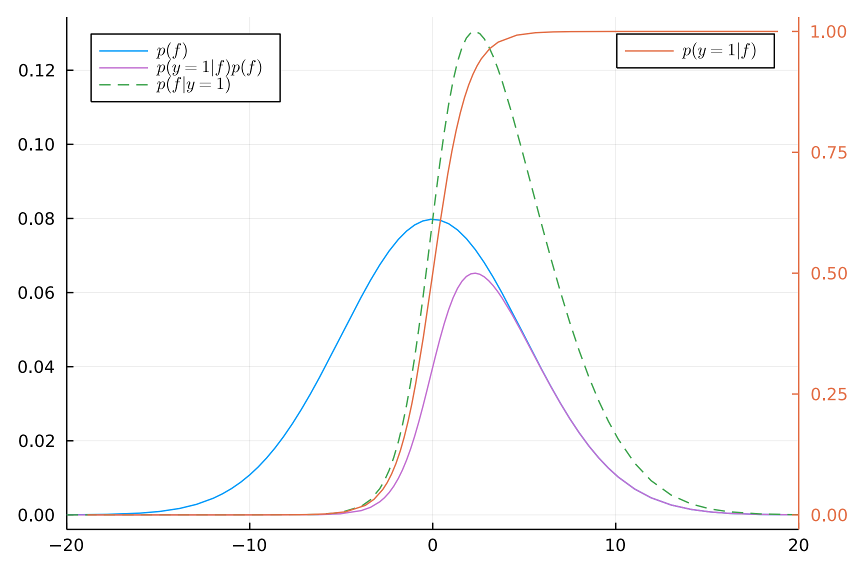
$$p_{\mathcal{N}}(\mathbf{f}) = \frac{1}{\sqrt{(2\pi)^k|\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{f}-\mu)^\top \Sigma^{-1}(\mathbf{f}-\mu)\right)$$

Approximate quadratic polynomial:
2nd-order Taylor expansion of log of $h(f) = p(y \mid f)p(f)$ at $\hat{f}$

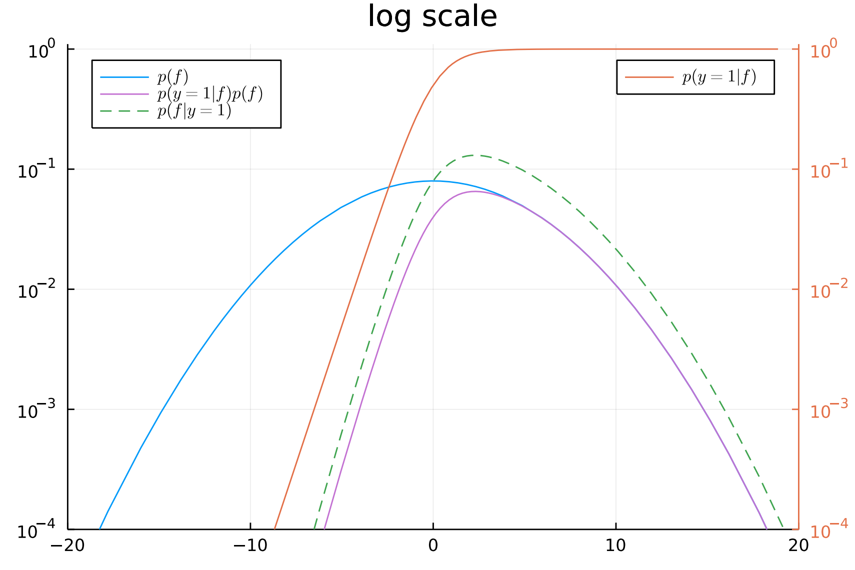
$$g(x+\delta) \approx g(x) + \left(\frac{\mathrm{d}g}{\mathrm{d}x}(x)\right)\delta + \frac{1}{2!}\left(\frac{\mathrm{d}^2 g}{\mathrm{d}x^2}(x)\right)\delta^2$$

1. Find mode of posterior
   2nd-order gradient optimisation (e.g. Newton's method)
2. Match curvature (Hessian) at mode

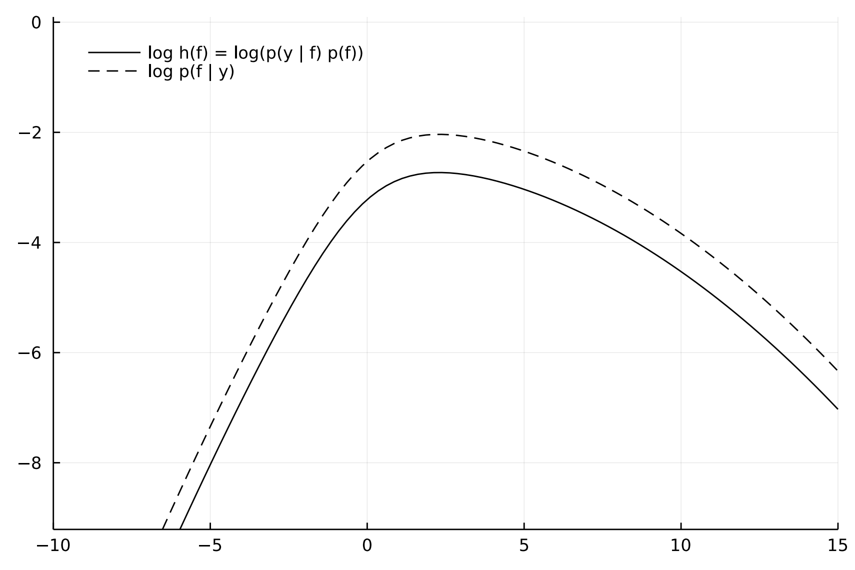
$p(f \mid y) = \frac{1}{Z} p(y \mid f) p(f)$



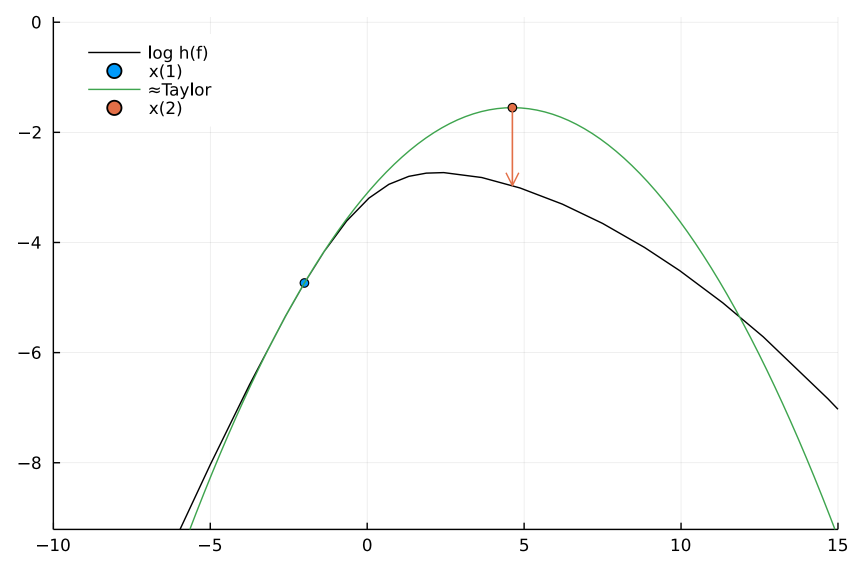
$\log p(f \mid y) = -\log Z + \log p(y \mid f) + \log p(f)$



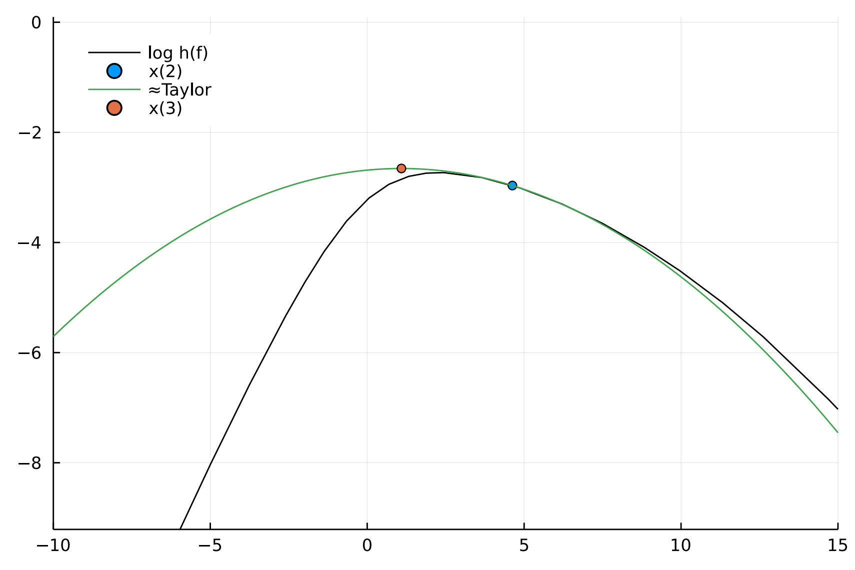
$\log p(f \mid y) = -\log Z + \log h(f)$



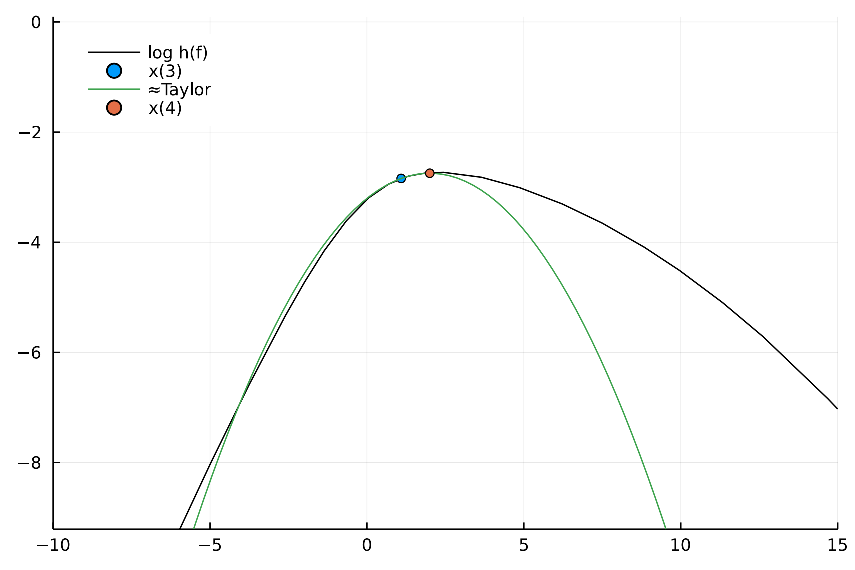
Newton's method



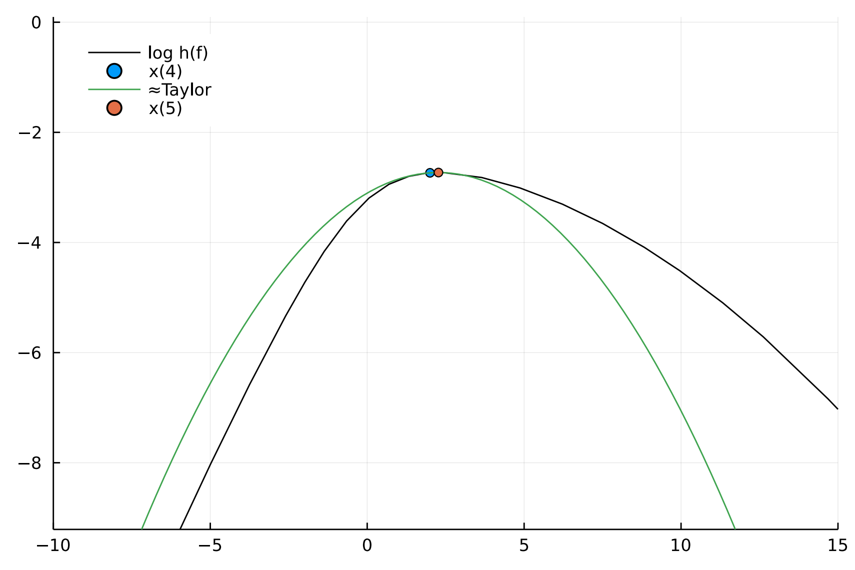
Newton's method



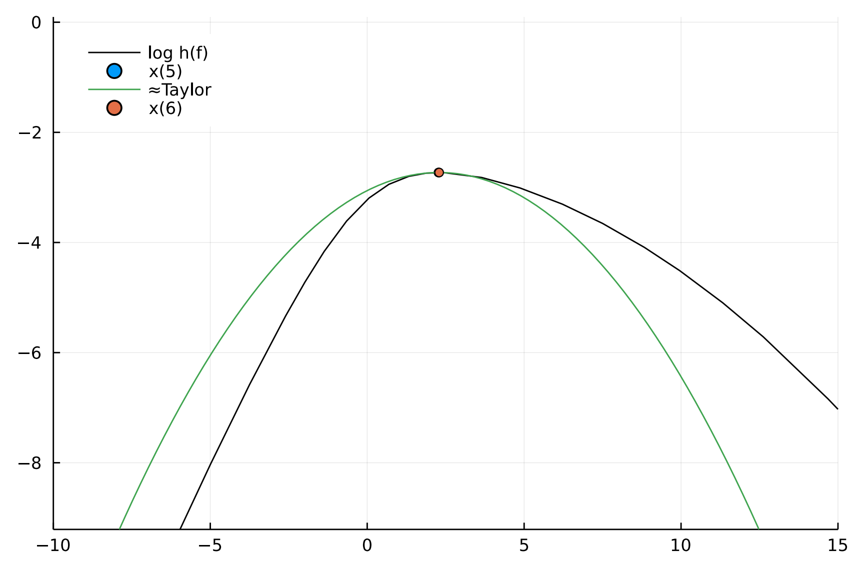
Newton's method



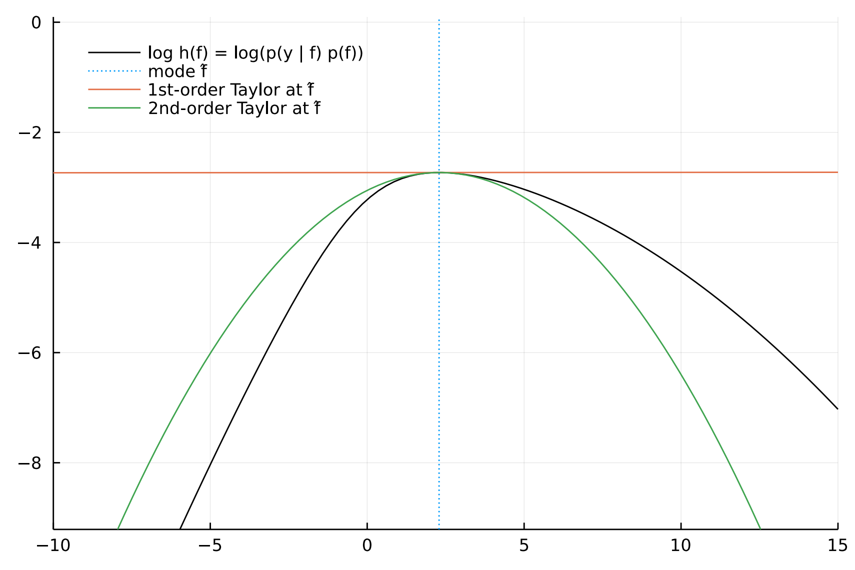
Newton's method



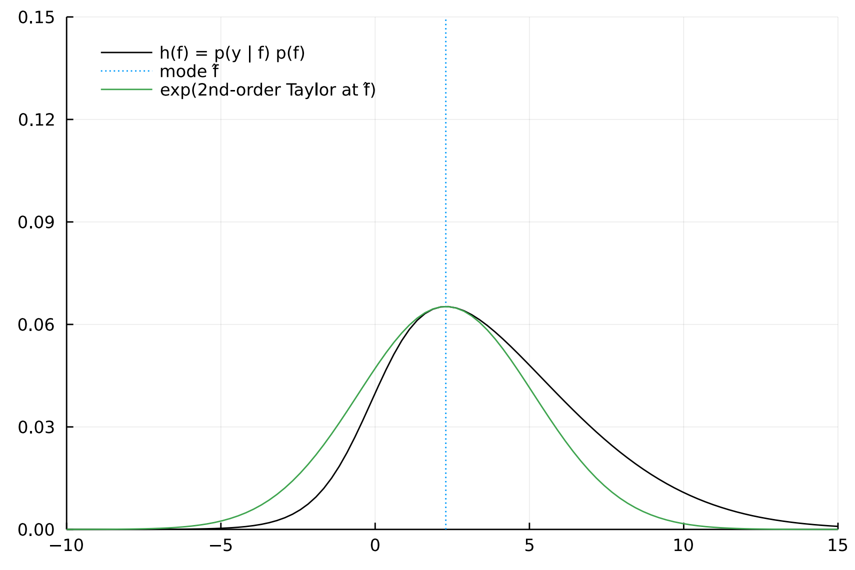
Newton's method



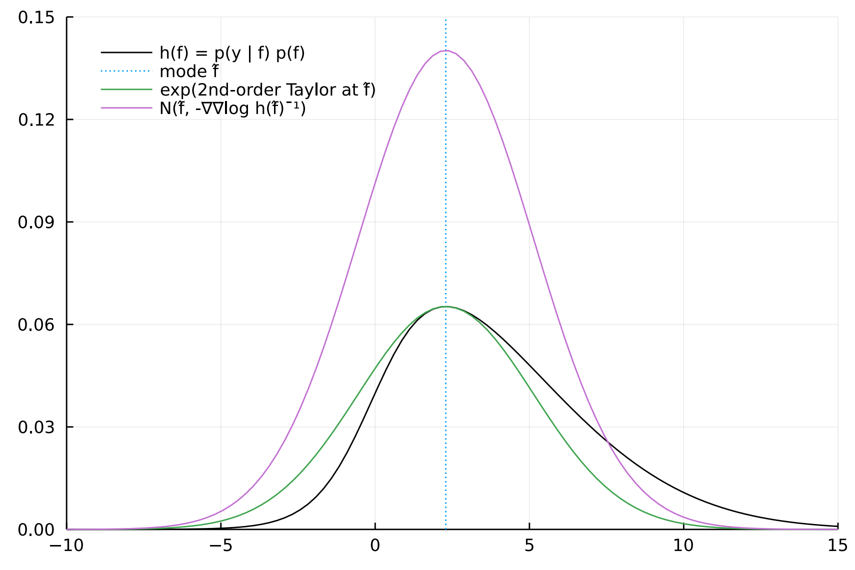
$\log p(f \mid y) + \log Z = \log h(f) \approx \mathcal{O}(f^2)$



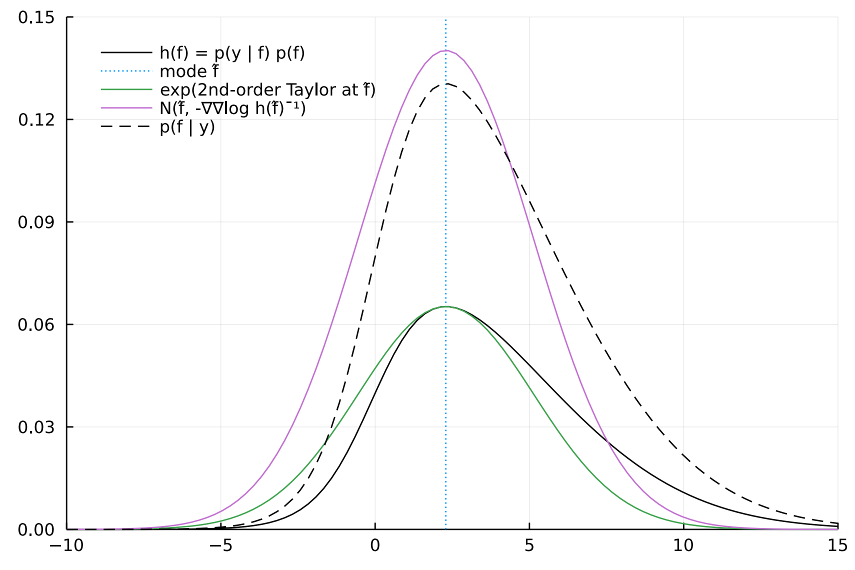
$p(f \mid y)\,Z \approx \exp(\mathcal{O}(f^2))$



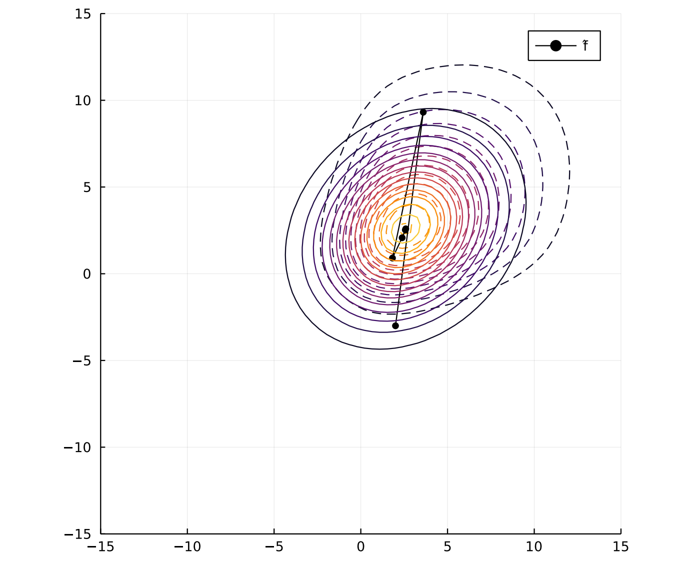
$p(f \mid y) \approx \mathcal{N}(f \mid \hat{f}, -\mathrm{d}^2 \log h/\mathrm{d}f^2)$



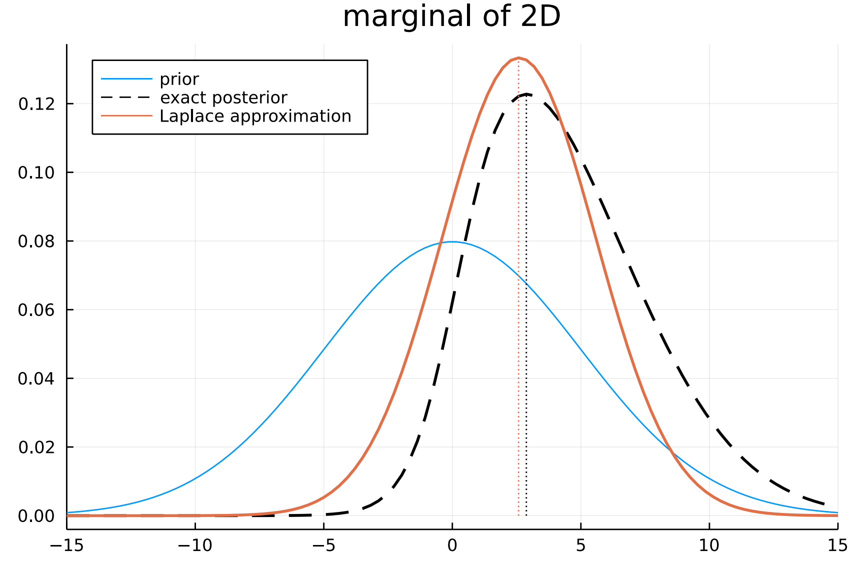
$p(f \mid y) \approx \mathcal{N}(f \mid \hat{f}, -\mathrm{d}^2 \log h/\mathrm{d}f^2) = q(f)$



Laplace in 2D example



Laplace in 2D: marginals



Laplace approximation: important properties

- find mode: Newton's method
- match curvature (Hessian) at mode
- "point estimate++"

+ simple, fast

– poor approximation if mode is not representative (e.g. Bernoulli)

– may not converge for non-log-concave likelihoods [3]

Choosing μ and Σ for $q(\mathbf{f})$

$$p(\mathbf{f} \mid \mathbf{y}) \approx q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mu =?, \Sigma =?)$$

match mean &
variance at point

minimise divergence

Laplace
approximation

Expectation
Propagation (EP)

Variational
Bayes (VB)

Minimising divergences

Kullback–Leibler (KL) divergence

“Relative entropy”, “information gain” *from q to p*

$$D_{\mathrm{KL}}(p\|q) = \mathrm{KL}[p(x)\|q(x)] = \mathbb{E}_{x\sim p}\Big[\log\frac{p(x)}{q(x)}\Big] = \int p(x)\Big[\log\frac{p(x)}{q(x)}\Big]\mathrm{d}x$$

- non-symmetric: $\mathrm{KL}[p\|q] \neq \mathrm{KL}[q\|p]$
- positive: $\mathrm{KL} \geq 0$ (Gibbs’ inequality)
- minimum: $\mathrm{KL}[p\|q] = 0 \Leftrightarrow q = p$.

Demo: KL between two Gaussians

Minimising divergences

$$p(\mathbf{f} \mid \mathbf{y}) \approx q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mu = ?, \Sigma = ?)$$

1. $\min \mathrm{KL}[p(\mathbf{f} \mid \mathbf{y}) \| q(\mathbf{f})]$**: Expectation Propagation**
2. $\min \mathrm{KL}[q(\mathbf{f}) \| p(\mathbf{f} \mid \mathbf{y})]$: Variational Bayes

Expectation Propagation (EP)

Expectation Propagation

Exact posterior:

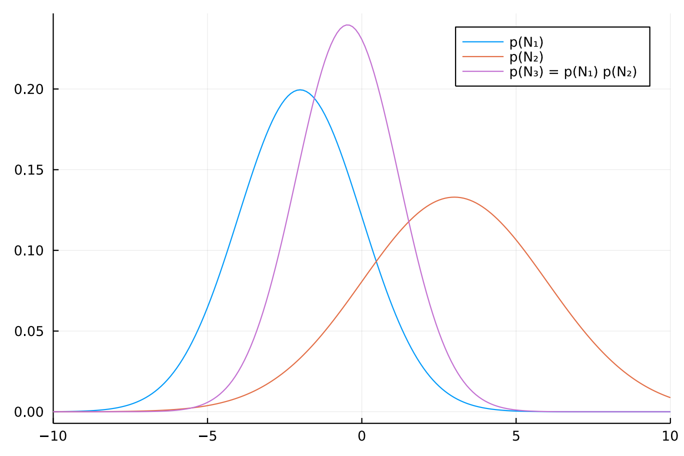
$$p(\mathbf{f} \mid \mathbf{y}) \propto p(\mathbf{f}) \prod_{i=1}^{N} p(y_i \mid f_i)$$

Approximate posterior:

$$q(\mathbf{f}) \propto p(\mathbf{f}) \prod_{i=1}^{N} t_i(f_i)$$

$$t_i = Z_i \mathcal{N}(f_i \mid \tilde{\mu}_i, \tilde{\sigma}_i^2)$$

Multiplying and dividing Gaussians



Adding and subtracting natural (canonical) parameters

Expectation Propagation iterations

“ $\min \mathrm{KL}[p(\mathbf{f} \mid \mathbf{y}) \| q(\mathbf{f})]$”

$$q(\mathbf{f}) \propto p(\mathbf{f}) \prod_{i=1}^{N} \underbrace{t_i(f_i)}_{\text{site } \propto \mathcal{N}(f_i)}$$

For each site i:

1. marginalize $\int q(\mathbf{f})\,\mathrm{d}f_{j\neq i} = q(f_i) \quad \not\propto t_i(f_i)$
2. improve local approximation: $\min \mathrm{KL}[q(f_i)\frac{p(y_i \mid f_i)}{t_i(f_i)} \| q(f_i)\frac{t_i'(f_i)}{t_i(f_i)}]$

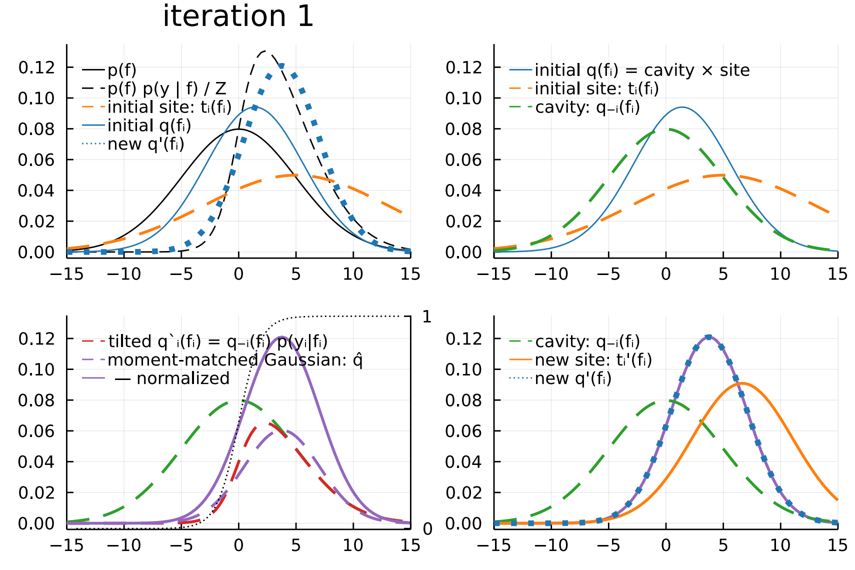
   2.1 *cavity* distribution $q_{-i}(f_i) = \frac{q(f_i)}{t_i(f_i)} \quad \Leftrightarrow \quad q(f_i) = q_{-i}(f_i)t_i(f_i)$

   2.2 *tilted* distribution $q_{\setminus i}(f_i) = q_{-i}(f_i)p(y_i \mid f_i)$

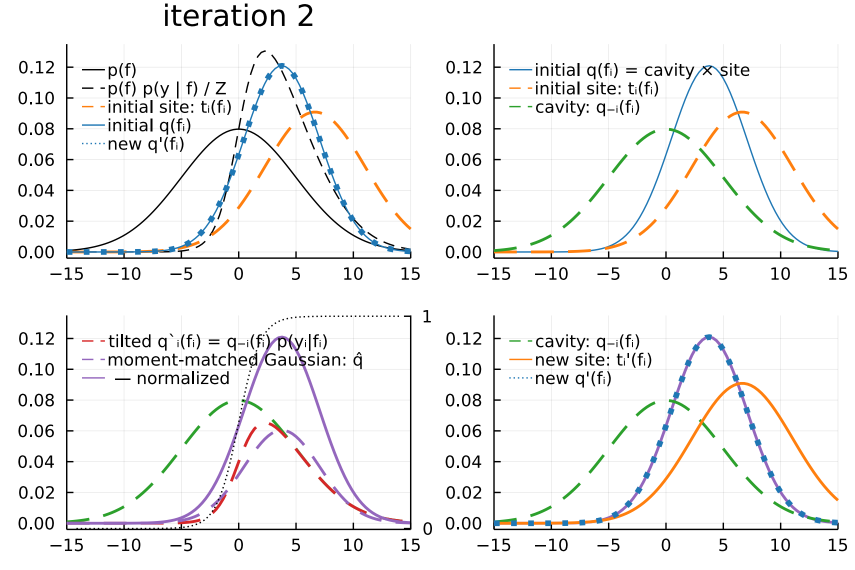
   2.3 $\operatorname{argmin} \mathrm{KL}[q_{-i}(f_i)p(y_i \mid f_i) \| \hat{q}]$ by moment-matching

   2.4 update site: $t_i'(f_i) = \frac{\hat{q}}{q_{-i}(f_i)} \quad \Leftrightarrow \quad \hat{q} = q_{-i}(f_i)\, t_i'(f_i)$
3. compute new $q'(\mathbf{f})$ (rank-1 update)

Expectation Propagation in 1D

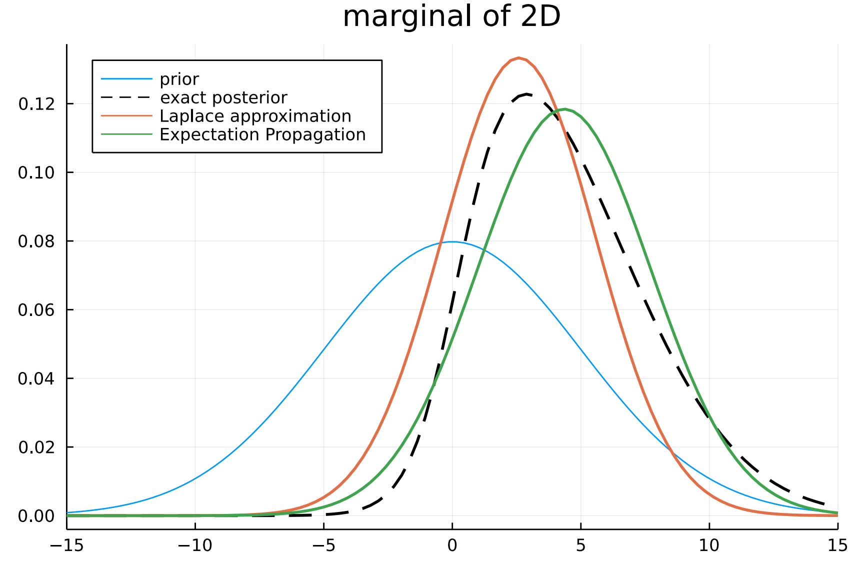


Expectation Propagation in 1D



Demo: EP in 2D

Marginals


marginal of 2D
prior
exact posterior
Laplace approximation
Expectation Propagation
0.12
0.10
0.08
0.06
0.04
0.02
0.00
−15
−10
−5
0
5
10
15

Expectation Propagation: important properties

- multiple passes required to converge
- moment-matching (e.g. covering multiple modes)

+ effective for classification

– not guaranteed to converge

– updates may be invalid (non-log-concave likelihoods)

Minimising divergences

$$p(\mathbf{f} \mid \mathbf{y}) \approx q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mu =?, \Sigma =?)$$

✓ $\min \mathrm{KL}[p(\mathbf{f} \mid \mathbf{y}) \| q(\mathbf{f})]$: Expectation Propagation

2. $\min \mathrm{KL}[q(\mathbf{f}) \| p(\mathbf{f} \mid \mathbf{y})]$**: Variational Bayes**

Variational Bayes (VB)
Variational Inference (VI)

Variational Bayes (VB)

Idea:
minimise divergence between $p(f \mid y)$ and $q(f)$ the “other” way

$$\operatorname*{argmin}_{\mu,\Sigma} \ \mathrm{KL}\left[q(f) \| p(f \mid y)\right]$$

Minimizing $\mathrm{KL}[q(f)\|p(f|y)]$

$$
\begin{aligned}
&\mathrm{KL}[q(f)\|p(f|y)]\\
&= \int q(f)\left[\log \frac{q(f)}{p(f\,|\,y)}\right]\mathrm{d}f = \int q(f)\left[\log q(f) - \log p(f\,|\,y)\right]\mathrm{d}f\\
&= \int q(f)\left[\log q(f) - \log p(f) - \log p(y\,|\,f) + \log p(y)\right]\mathrm{d}f\\
&= \int q(f)\left[\log \frac{q(f)}{p(f)}\right]\mathrm{d}f - \int q(f)\left[\log p(y\,|\,f)\right]\mathrm{d}f + \log p(y)\\
&= \mathrm{KL}[q(f)\|p(f)] - \int q(f)\left[\log p(y\,|\,f)\right]\mathrm{d}f + \log p(y)
\end{aligned}
$$

$$
\log p(y) = \int q(f)\left[\log p(y\,|\,f)\right]\mathrm{d}f - \mathrm{KL}[q(f)\|p(f)] + \mathrm{KL}[q(f)\|p(f|y)]
$$

ELBO

$$\begin{aligned}\log p(y) &= \int q(f)\left[\log p(y\,|\,f)\right]\mathrm{d}f - \mathrm{KL}[q(f)\|p(f)] + \mathrm{KL}[q(f)\|p(f|y)] \\ &\geq \int q(f)\left[\log p(y\,|\,f)\right]\mathrm{d}f - \mathrm{KL}[q(f)\|p(f)]\end{aligned}$$

Lower bound on the (log-)evidence $p(y)$ = ELBO

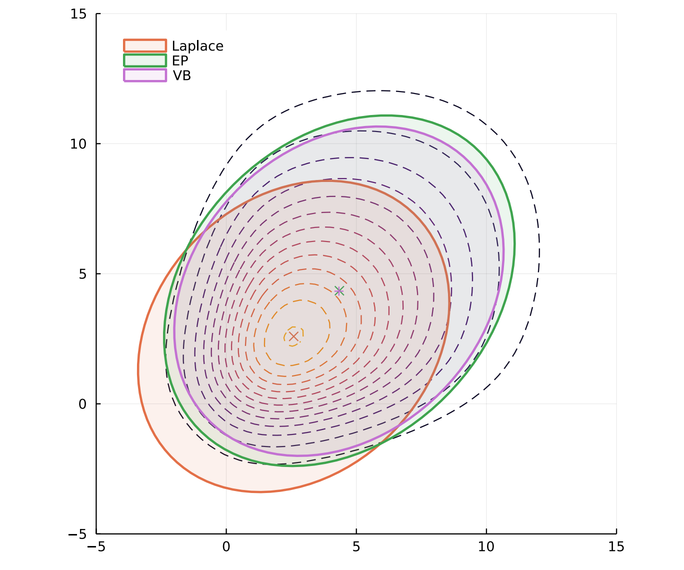
Likelihood term

$$\int q(\mathbf{f})\left[\log p(\mathbf{y} \mid \mathbf{f})\right]\mathrm{d}\mathbf{f}$$

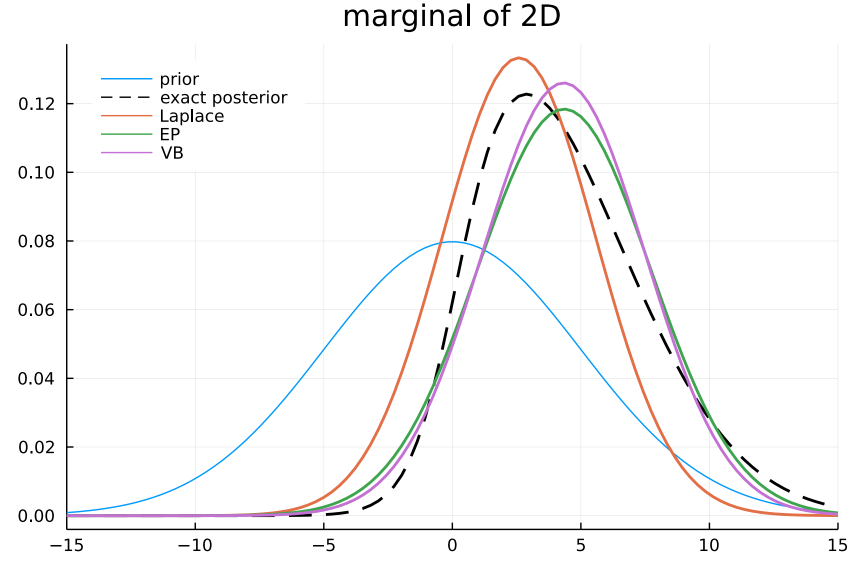
$$\sum_{i=1}^{N}\int q(f_i)\left[\log p(y_i \mid f_i)\right]\mathrm{d}f_i$$

- analytic (e.g. Exponential, Gamma, Poisson)
- Gauss–Hermite quadrature
- Monte Carlo (e.g. multi-class classification)

Comparison 2D



Marginals



marginal of 2D
prior
exact posterior
Laplace
EP
VB
0.12
0.10
0.08
0.06
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0.02
0.00
−15
−10
−5
0
5
10
15

Variational Bayes: important properties

- principled: directly minimising divergence from true posterior
- mode-seeking (e.g. multi-modal posterior: fits just one)

+ minimises a true lower bound → convergence

– underestimates variance

Outline

- ✓ Gaussian processes with Gaussian likelihood
- ✓ What is the likelihood? Connecting observations and Gaussian process prior
- ✓ Non-Gaussian likelihoods: what happens to the posterior?

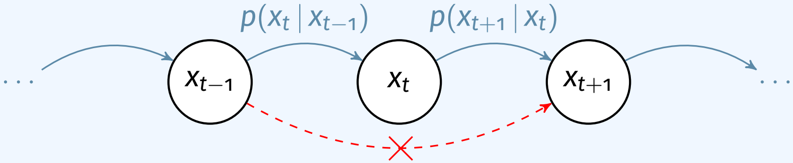
4. **How to approximate the intractable**
   - ✓ with Gaussians
     - ■ Laplace
     - ■ Expectation Propagation
     - ■ Variational Bayes

   4.2 **with samples: MCMC**

5. Comparisons

Markov Chain Monte Carlo

Markov Chain



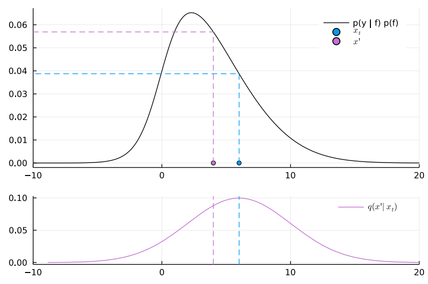
- Samples $x_1, \ldots, x_T$
- “Markov” = 1-step history
- $x_{t+1} \sim p(x_{t+1} \mid x_t)$, independent of $x_{t-1}, \ldots, x_1$

Markov Chain Monte Carlo (MCMC)

Generate samples $\{x_t\} \sim p(f \mid y)$

Requires:

- *unnormalized* posterior $h(f) = p(y \mid f)p(f)$
- Markov proposal $q(x' \mid x_t)$
- initial x_0



In each iteration t:

1. Random proposal $x' \sim q(x' \mid x_t)$
2. Acceptance probability $\frac{h(x')}{h(x_t)}$

accept: $x_{t+1} = x'$ reject: copy $x_{t+1} = x_t$

$h(x') > h(x_t)$: always accepts → climbs uphill

Demo: MCMC in 2D

MCMC: IMPORTANT PROPERTIES

- burn-in
- acceptance ratio
- auto-correlation, effective sample size (ESS); thinning to save memory
- mixing and multiple chains ($\hat{R}$)
- better proposals (HMC, NUTS)

+ very accurate (gold-standard)

– very slow, predictions require keeping all (thinned) samples around

Michael Betancourt's `betanalpha.github.io/writing/`

MCMC: ROBUST IMPLEMENTATIONS

- Stan
- PyMC3
- TensorFlow Probability (GPflow)
- Turing.jl

Comparison

Comparison

MCMC

- samples
- gold standard
- slow

Laplace

- $\mathcal{N}$ = curvature at mode
- simple & fast
- often poor approximation

EP

- $\mathcal{N}$ matches marginal moments
- good calibration in classification
- may not converge

Variational Bayes

- $\mathcal{N}$ minimises $\mathrm{KL}[q(f)\|p(f \mid y)]$
- principled, any likelihood
- underestimates variance

What we did not cover...

- Marginal likelihood approximations for hyperparameter learning [6]
- How parametrisation affects Gaussianity of $p(f \mid y)$
- Connections between EP and VB ("PowerEP") [1]
- Combinations of MCMC and variational methods
- Augmenting likelihood with auxiliary variable $\rightarrow$ conditionally conjugate model [2]

Questions!

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