

Gaussian processes for non-Gaussian likelihoods

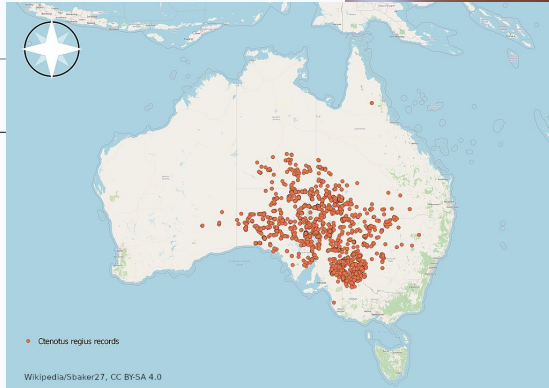
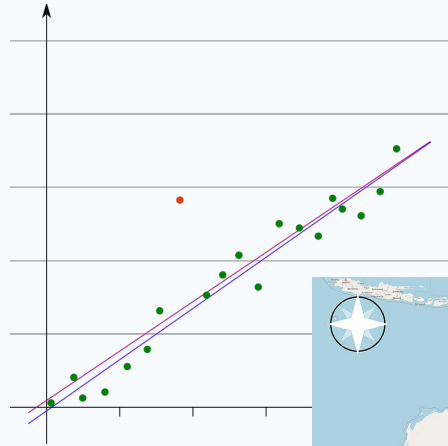
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Finnish Center for Artificial Intelligence
& Aalto University

LIKE2022 winter school, 10 January 2022

Not Gaussian noise



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. Comparison

- + *Intuitive* understanding
- + Learning the language

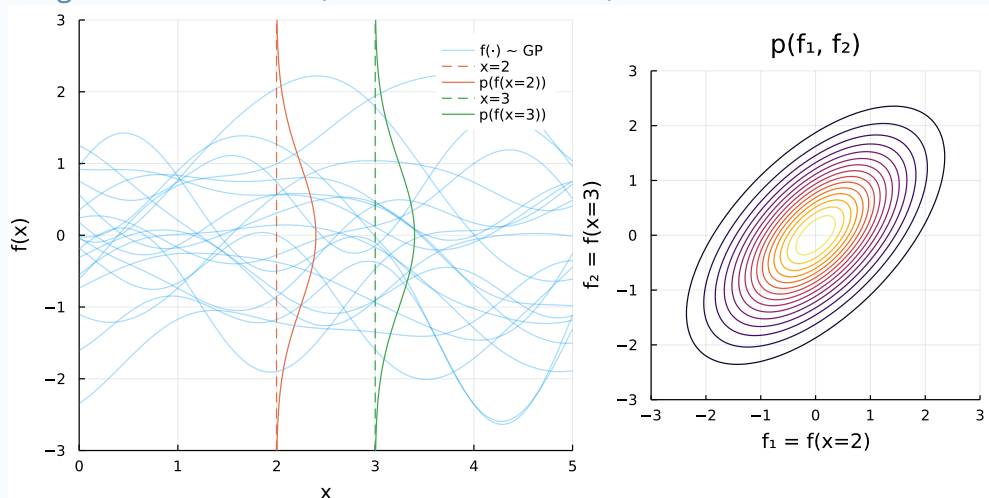
- In-depth expertise
- Lots of maths

Setting the scene

Gaussian process $f(\cdot)$

Distribution over functions

Marginals are Gaussian (mean and covariance)

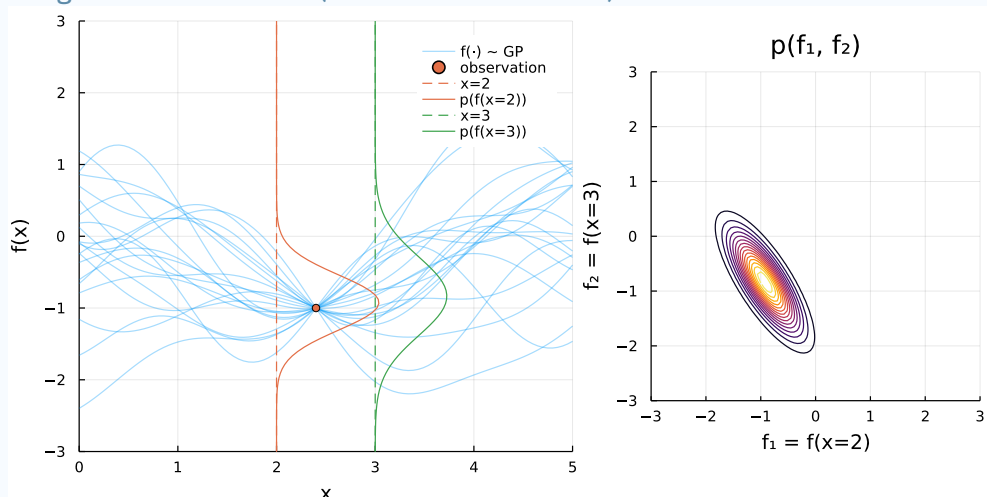


infinitecuriosity.org/vizgp

Gaussian process conditioned on observation

Distribution over functions

Marginals are Gaussian (mean and covariance)

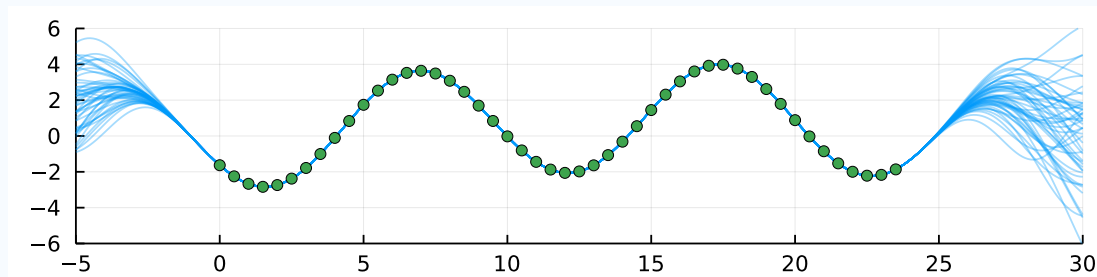


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exact conditioning

Without noise model, we interpolate observations:

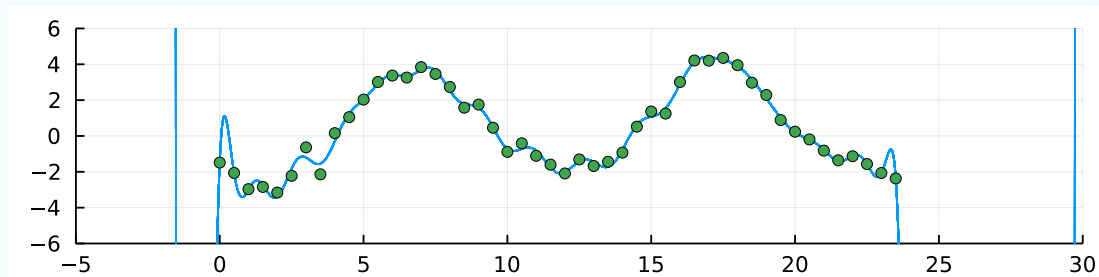
$$y(x) = f(x) + \epsilon, \quad \epsilon \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_{\text{noise}}^2)$$
$$p(y|f) = \mathcal{N}(y|f, \sigma_{\text{noise}}^2)$$



exact conditioning

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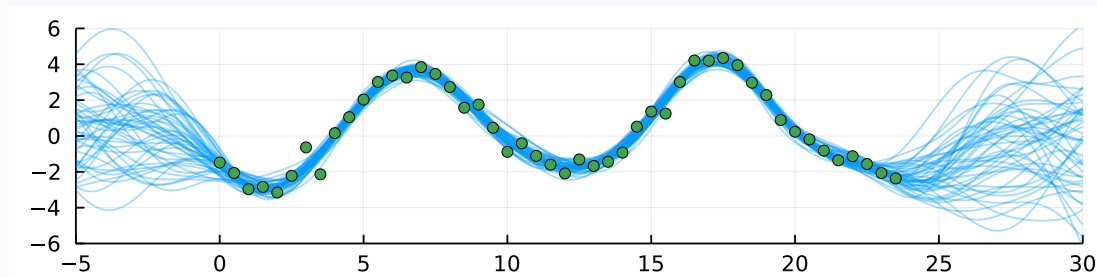
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Gaussian noise model

Gaussian additive noise model, written two ways:

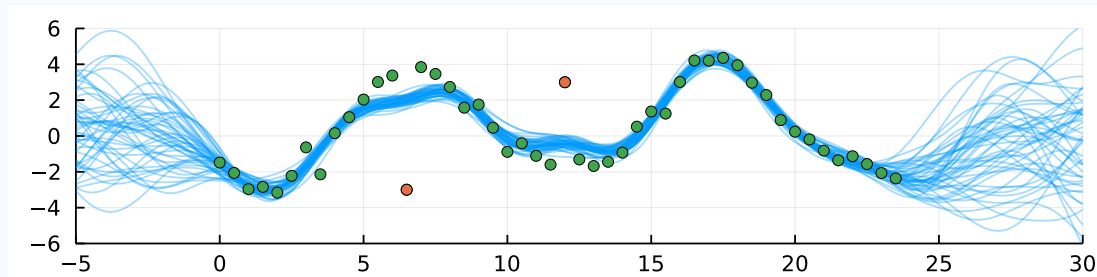
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misspecified Gaussian noise model

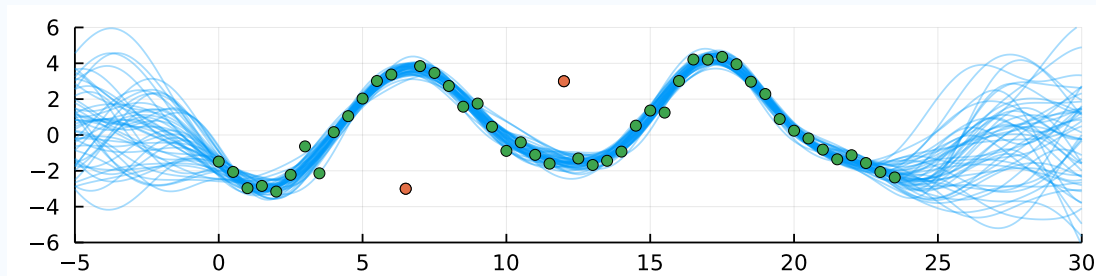
Gaussian additive noise model, written two ways:

$$y(x) = f(x) + \epsilon, \quad \epsilon \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_{\text{noise}}^2)$$
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heavy-tailed noise model

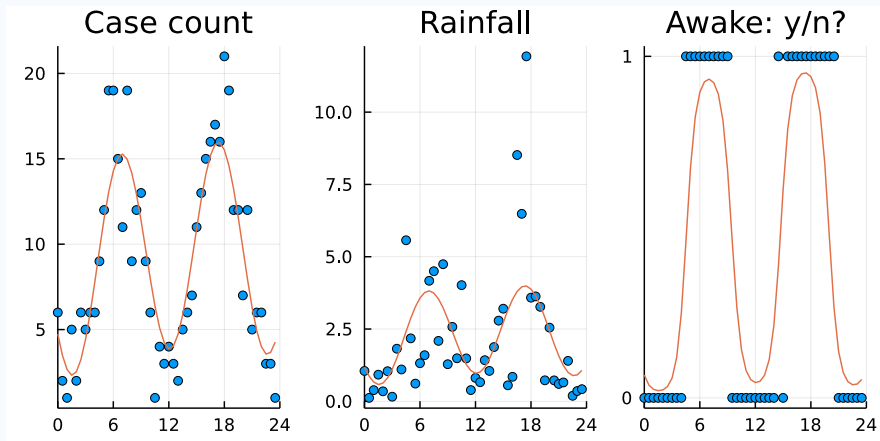
$$y(x) = f(x) + \epsilon, \quad \epsilon \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_{\text{noise}}^2)$$
$$p(y|f) = \mathcal{N}(y|f, \sigma_{\text{noise}}^2)$$



- ✓ 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?
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Likelihood

Non-Gaussian observations



latent functional relationship
 $p(y_i | f(x_i))$

Likelihood

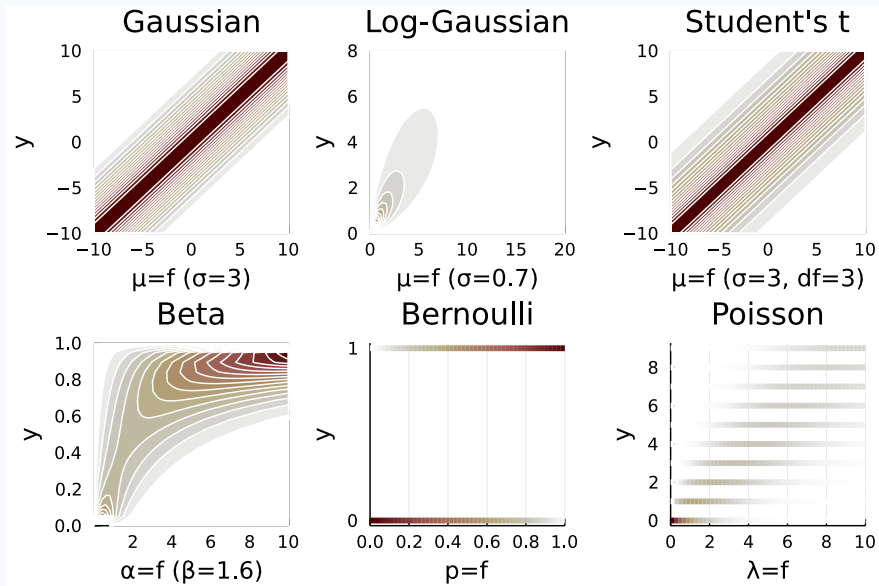
$$p(\mathbf{y} | \mathbf{f}) = \prod_{i=1}^N p(y_i | f_i); \quad f_i = f(x_i)$$

factorizing

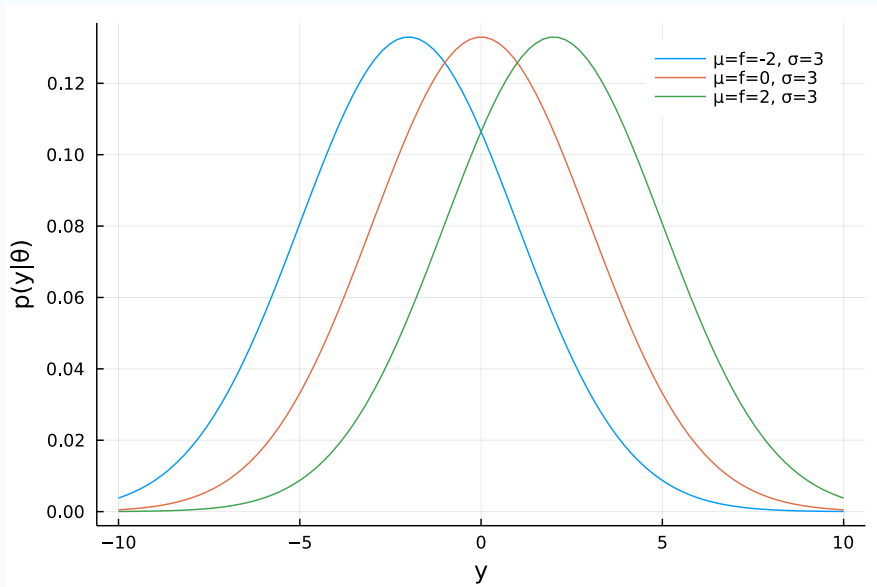
$$p(y | f)$$

Function of two arguments:

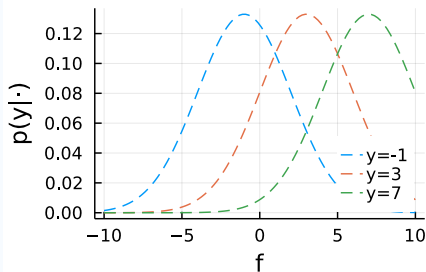
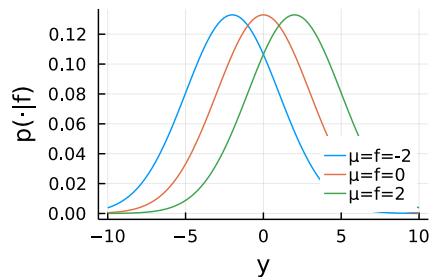
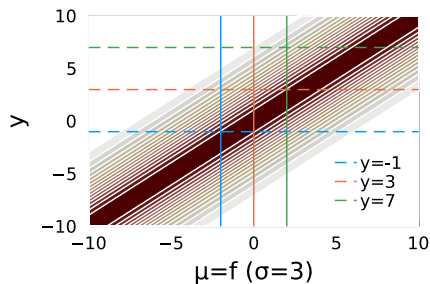
$$y \mapsto p(y | f), \quad f \mapsto p(y | f)$$



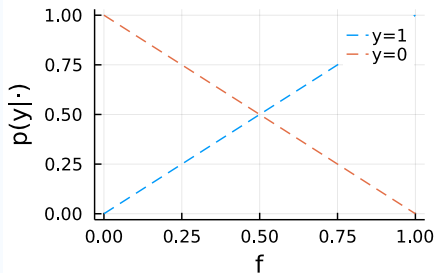
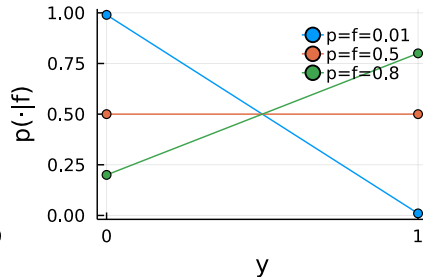
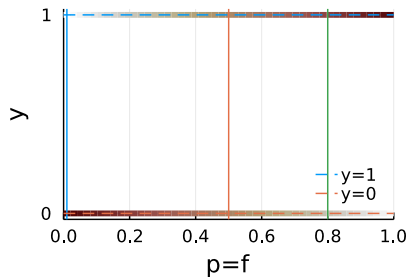
$p(y | f)$: Gaussian



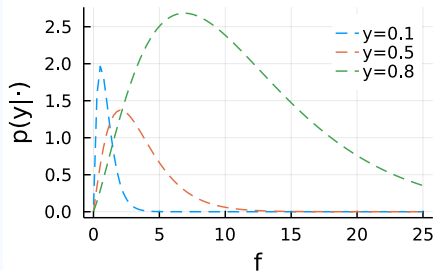
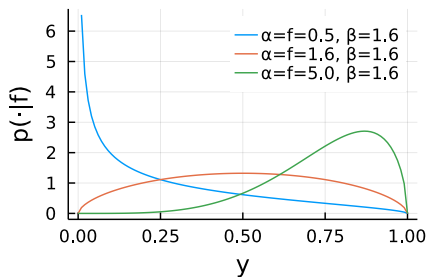
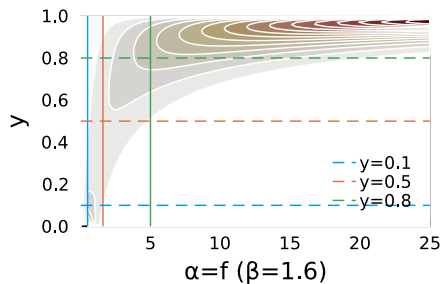
$p(y | f)$: Gaussian

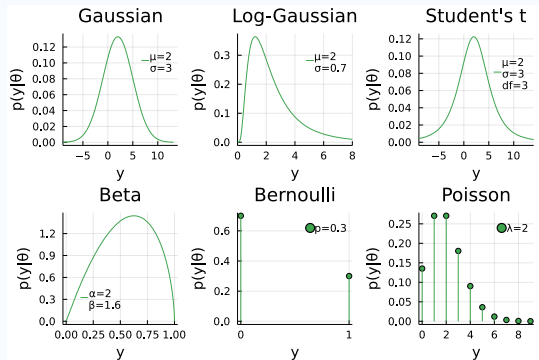
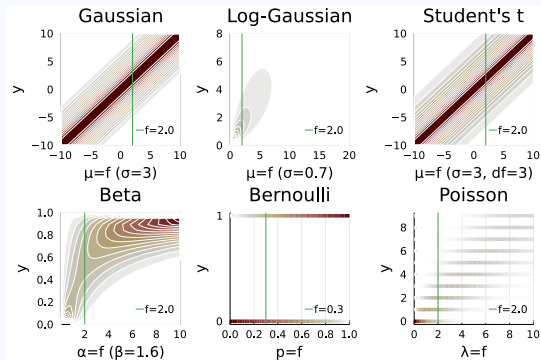


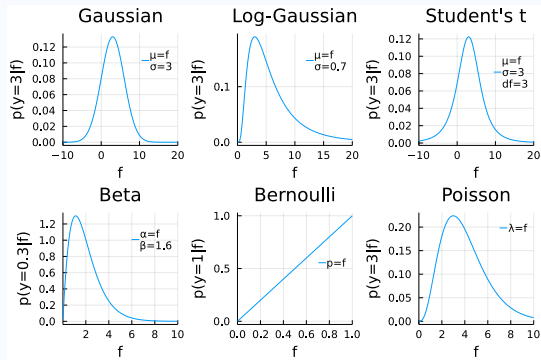
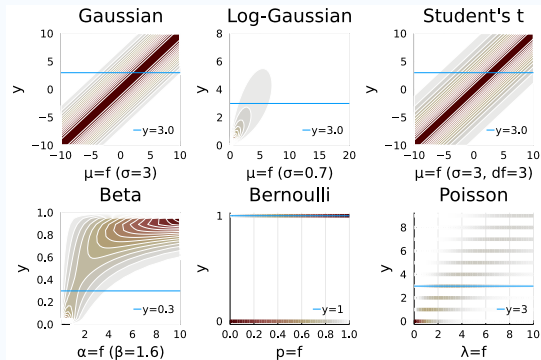
$p(y | f)$: Bernoulli



$p(y | f)$: Beta







Two aspects of likelihoods:

1. link functions
2. log-concavity

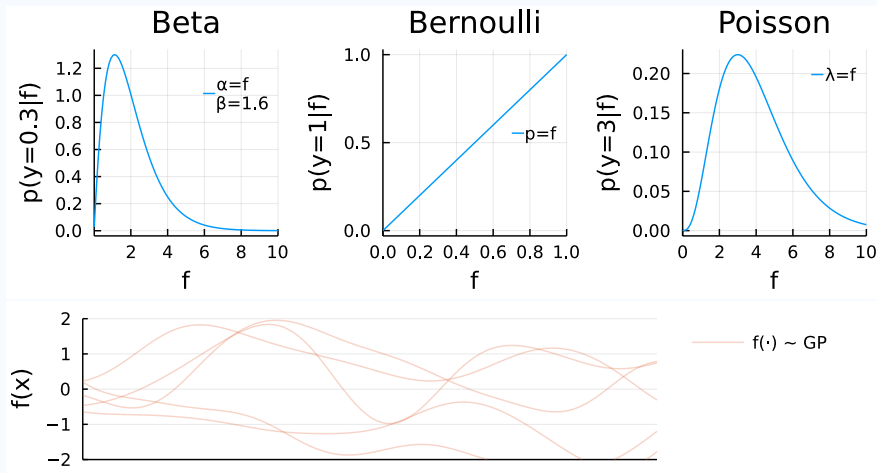
Link functions

$$\mathbb{E}[y] = \theta \in (0 \dots \infty)$$

$$f \sim \mathcal{N} \quad \in (-\infty \dots \infty)$$

$$\text{link}(\theta) = f$$

$$\theta = \text{invlink}(f)$$



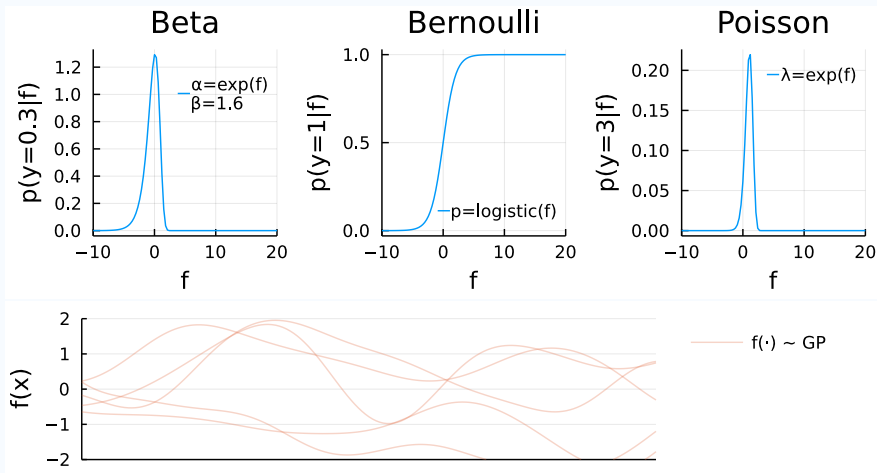
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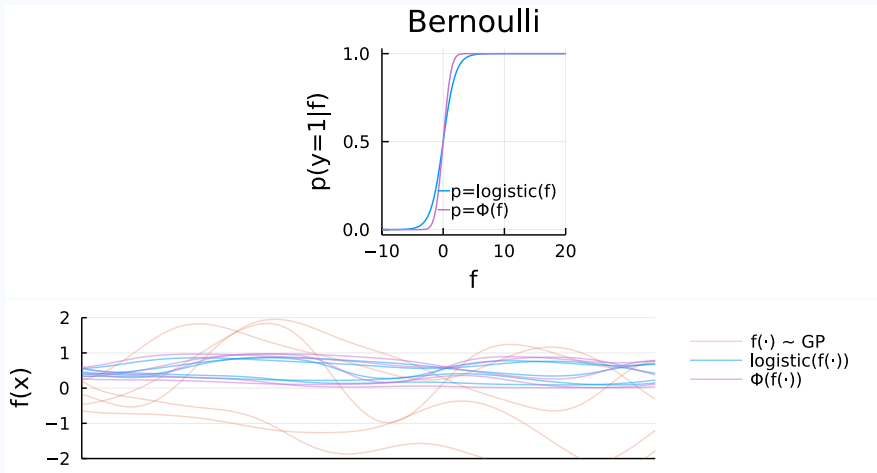
Link functions

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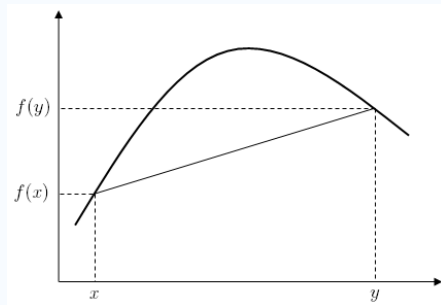
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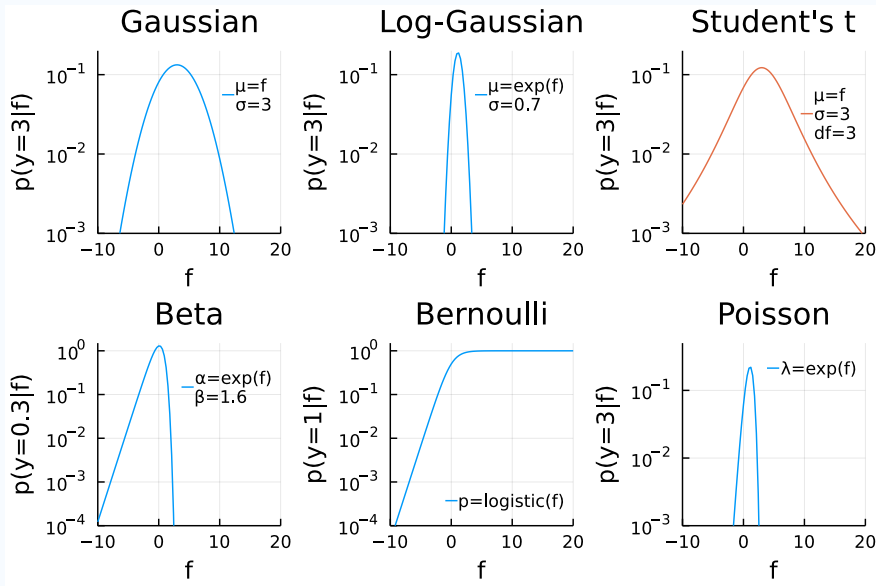


(Log-)concavity



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

Log-concavity of likelihoods



- ✓ 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
- 5. Comparison

Posterior

Likelihood

$$p(y | f)$$

Joint distribution

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

Posterior

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

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

Posterior predictions

At new point x^* :

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

At training data:

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

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

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

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

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

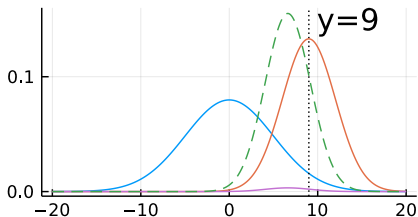
Gaussian (process) prior $p(f(\cdot)) \dots$

& Gaussian likelihood: conjugate case \rightarrow posterior Gaussian

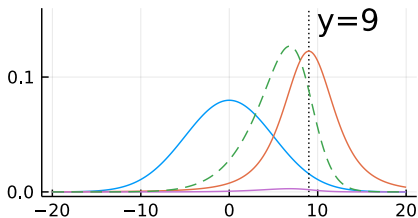
& **non**-Gaussian $p(y|f) \rightarrow p(\mathbf{f} | \mathbf{y})$ also **non**-Gaussian, **intractable**

1D examples

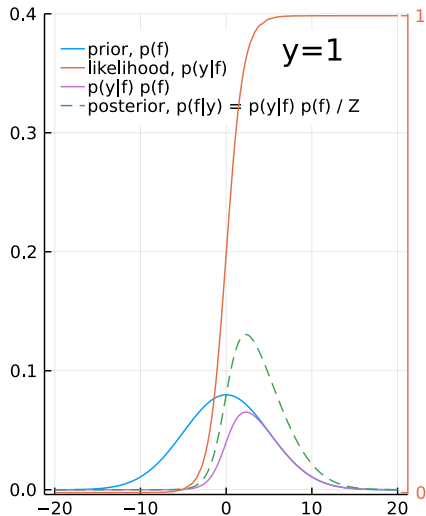
Gaussian



Student's t

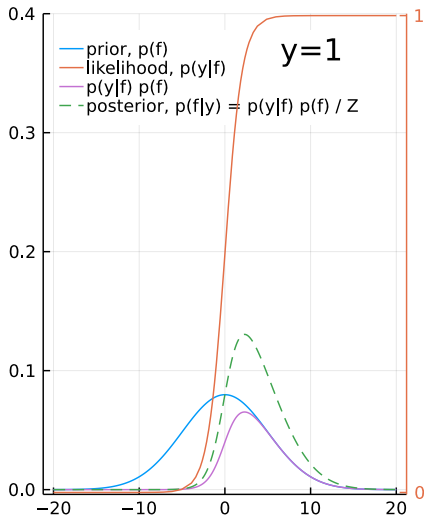


Bernoulli

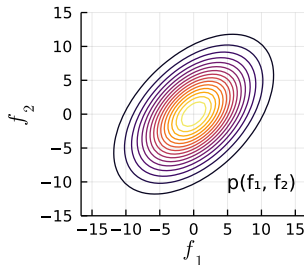


Bernoulli example in 2D

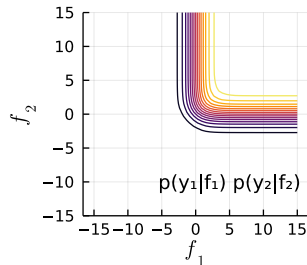
Bernoulli



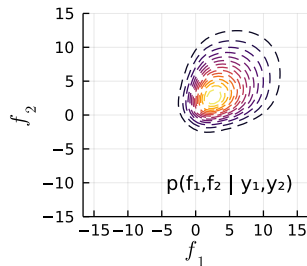
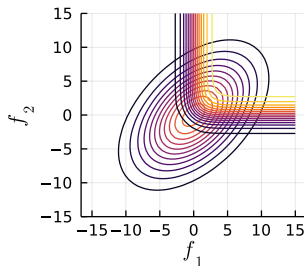
Prior



Likelihood



Posterior



Posterior for N observations

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

$$f_1 = f(x_1)$$

$$f_2 = f(x_2)$$

$$\vdots$$

$$f_N = f(x_N)$$

Summary so far

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

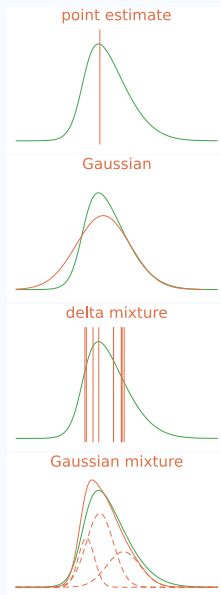
Questions?! :)

- ✓ 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. Comparison

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:

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

Predictions at new points:

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

Demo: What does this mean for Gaussian processes?

tinyurl.com/nongaussian-inference-viz-v1

Choosing μ and Σ for $q(\mathbf{f})$

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

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

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

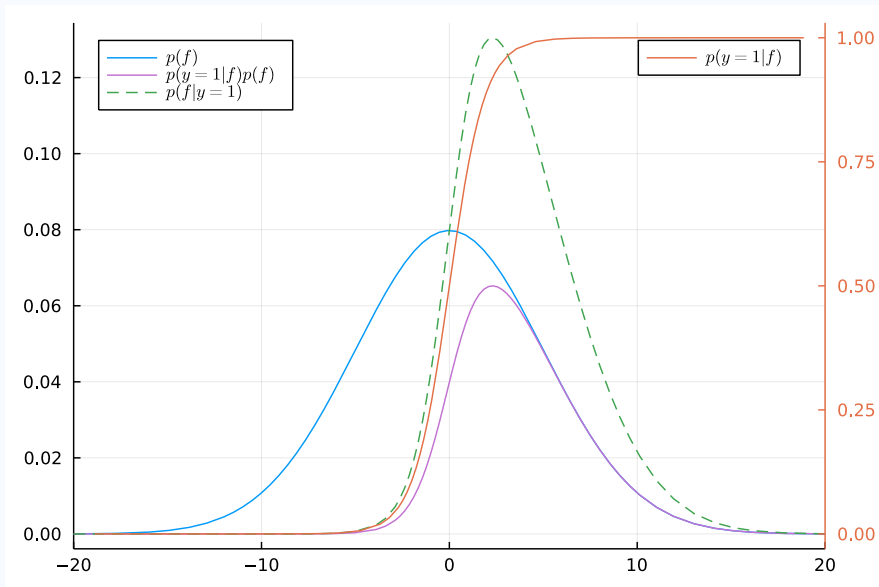
quadratic polynomial through approximation:

2nd-order Taylor expansion of log of $h(f) = p(y|f)p(f)$ at \hat{f}

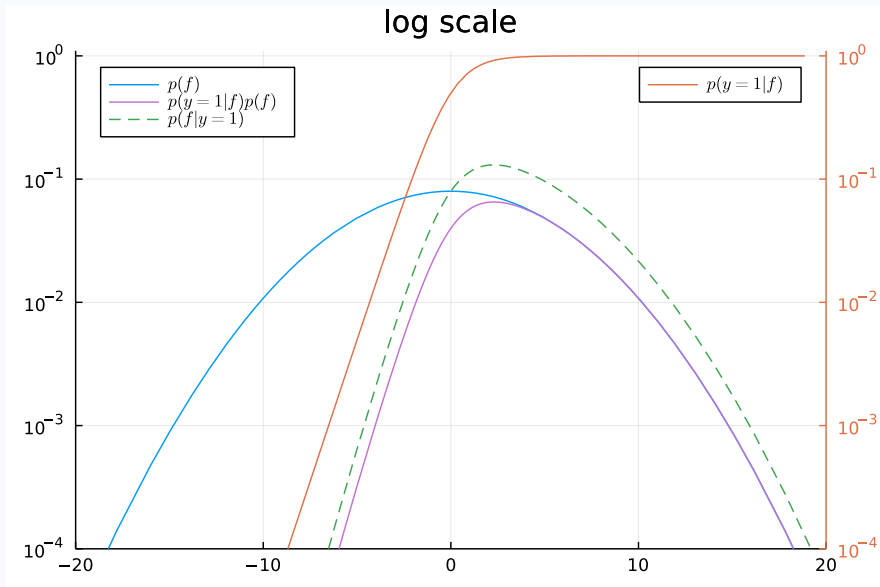
$$g(x + \delta) \approx g(x) + \left(\frac{dg}{dx}(x)\right)\delta + \frac{1}{2!}\left(\frac{d^2g}{dx^2}(x)\right)\delta^2$$

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

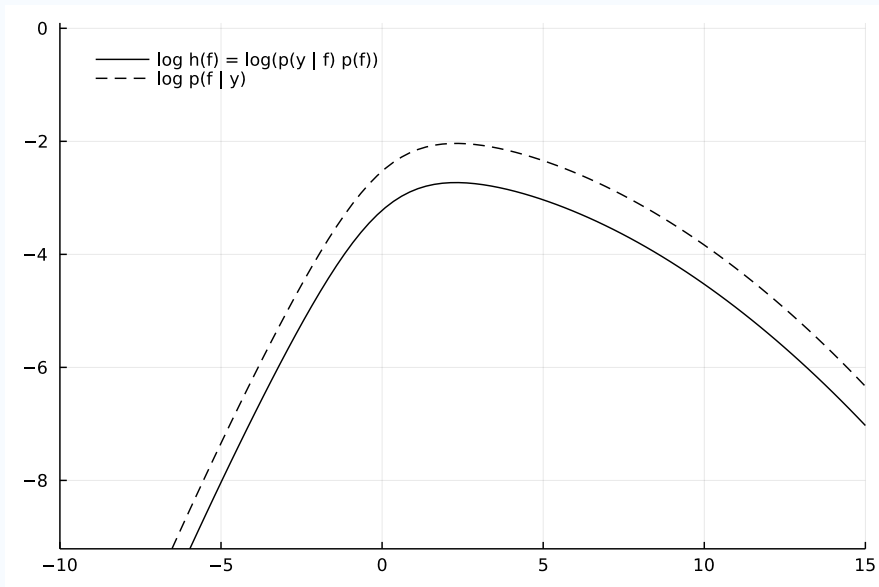
$$p(f|y) = \frac{1}{Z} p(y|f)p(f)$$



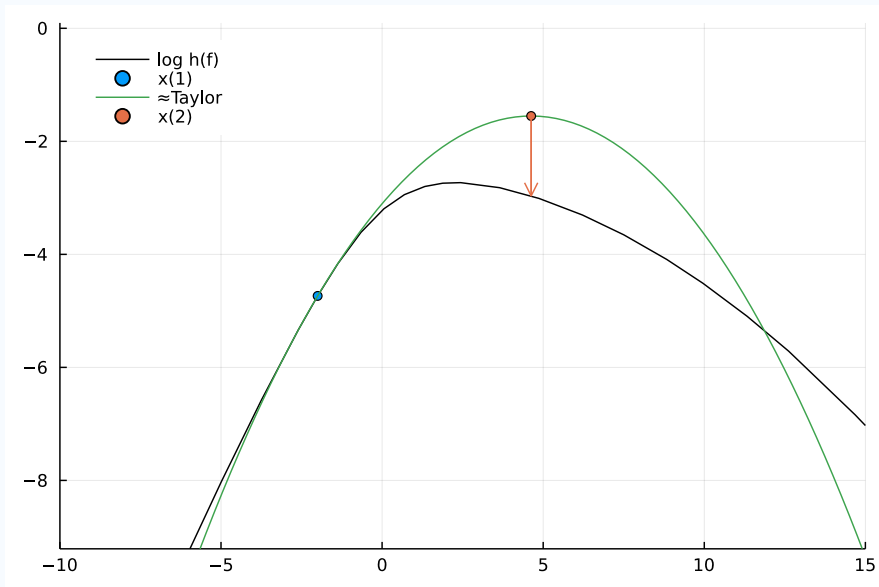
$$\log p(\mathbf{f} | \mathbf{y}) = -\log \mathbf{Z} + \log p(\mathbf{y} | \mathbf{f}) + \log p(\mathbf{f})$$



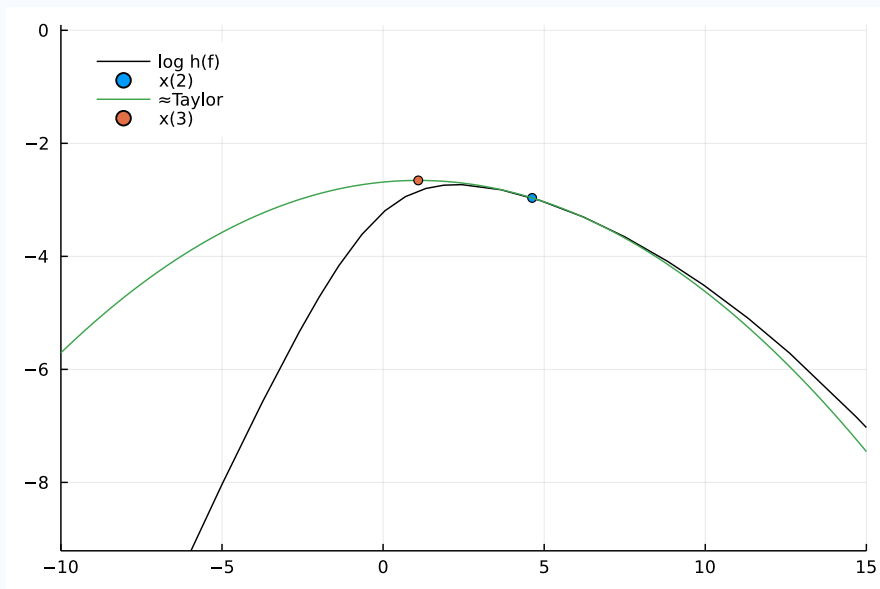
$$\log p(f | y) = -\log Z + \log h(f)$$



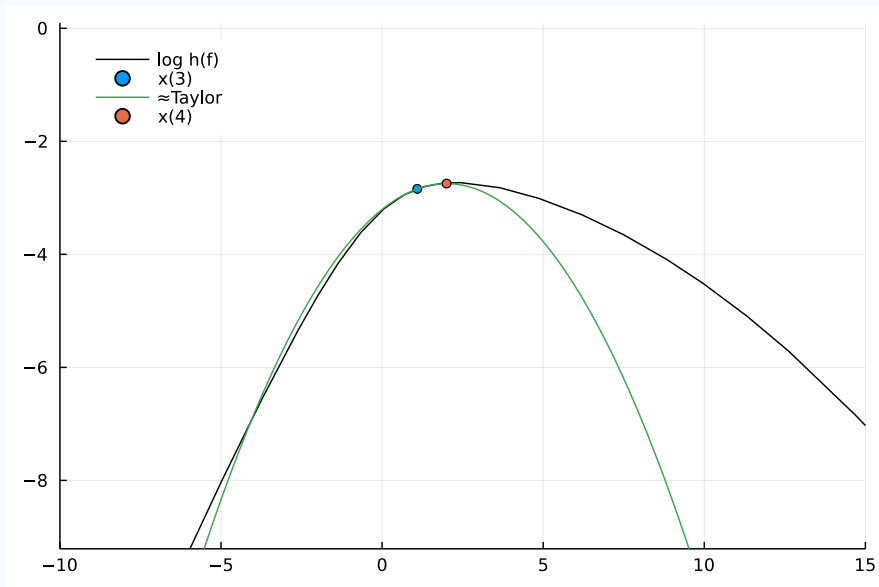
Newton's method



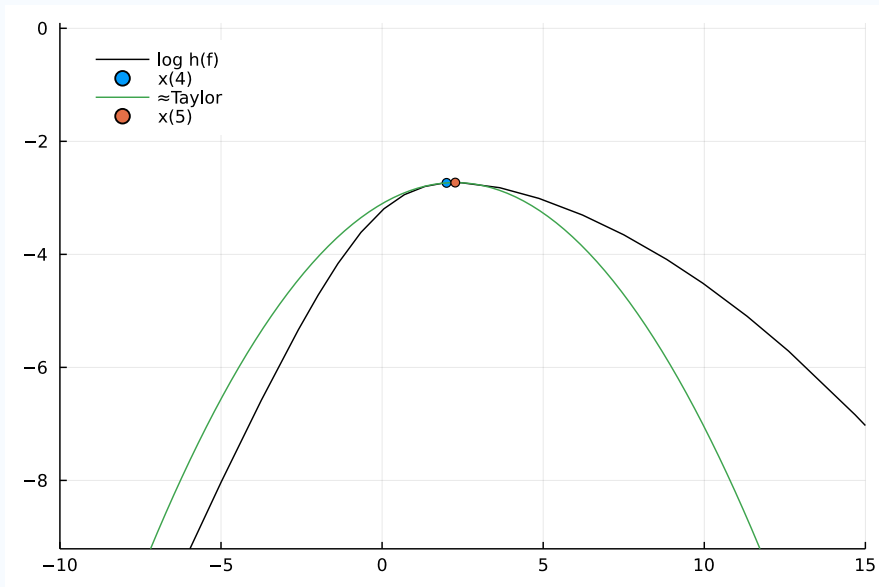
Newton's method



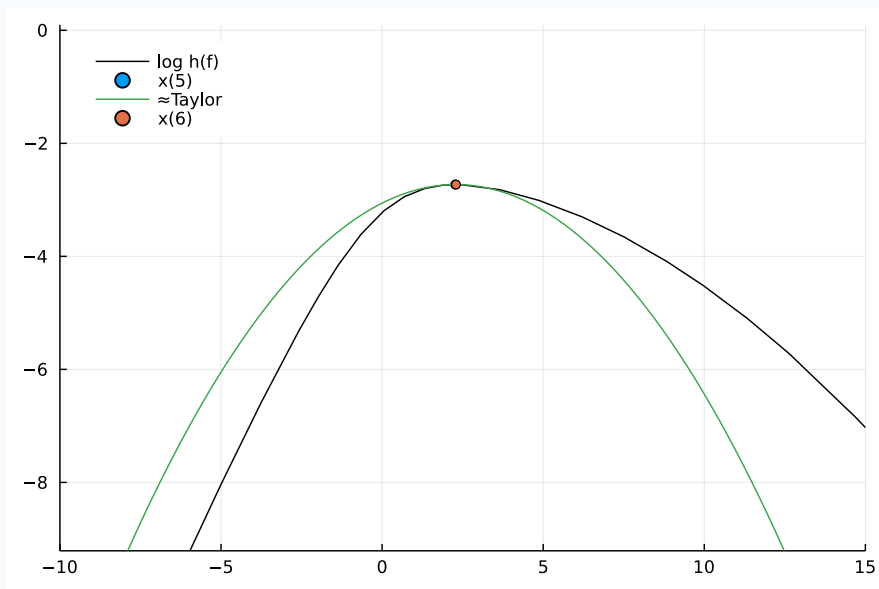
Newton's method



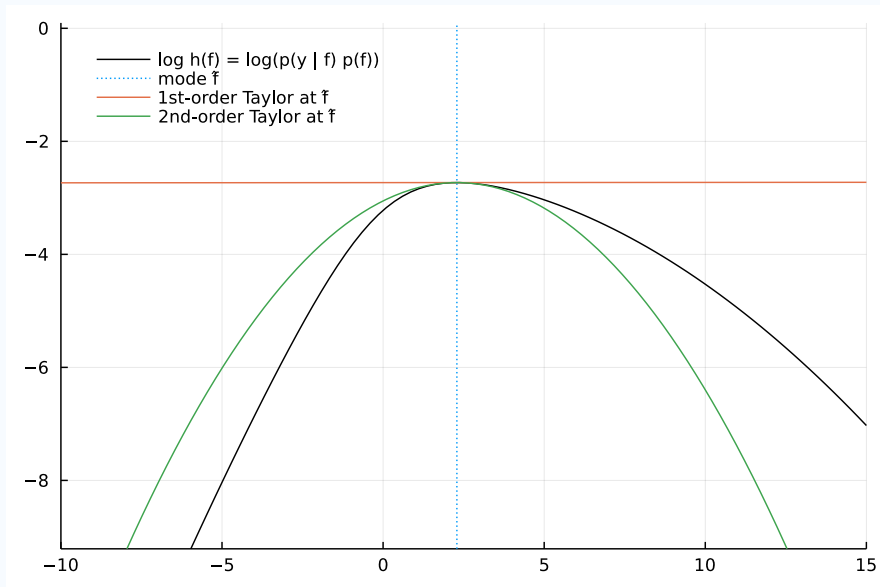
Newton's method



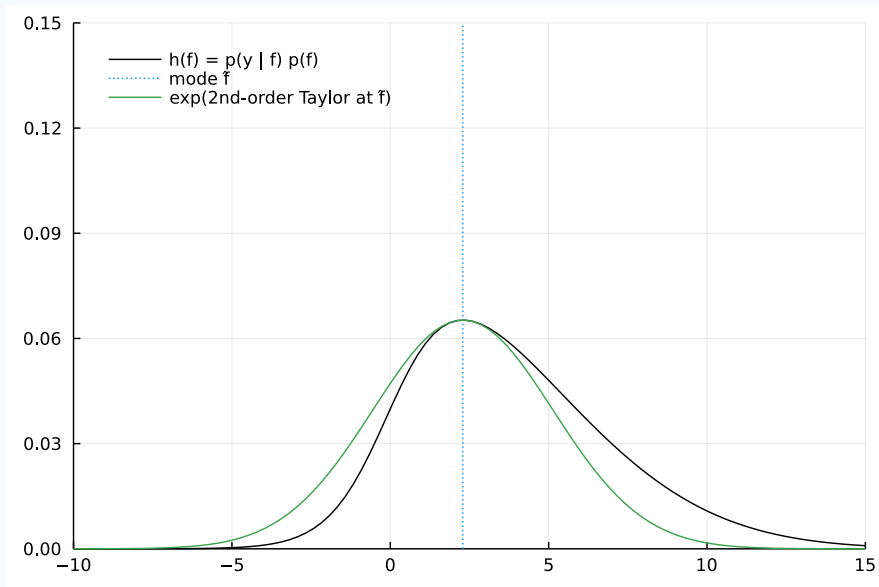
Newton's method



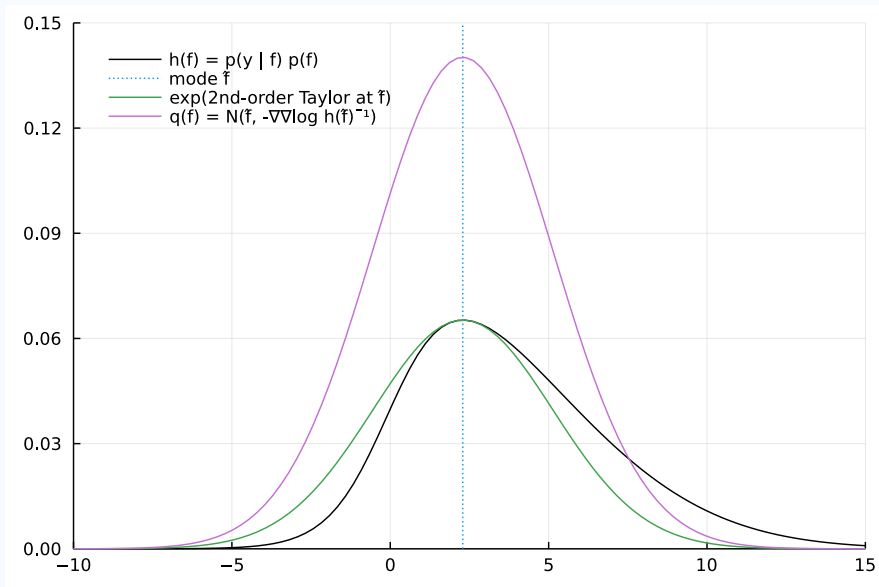
$$\log p(\textcolor{red}{f} \mid \textcolor{red}{y}) + \log \textcolor{red}{Z} = \log h(f) \approx \mathcal{O}(f^2)$$



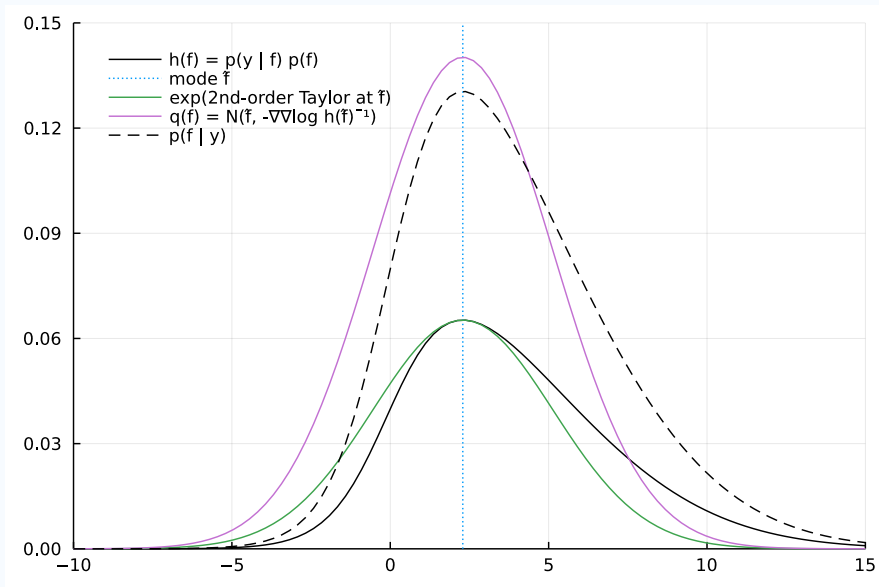
$$p(f | y) Z \approx \exp(\mathcal{O}(f^2))$$



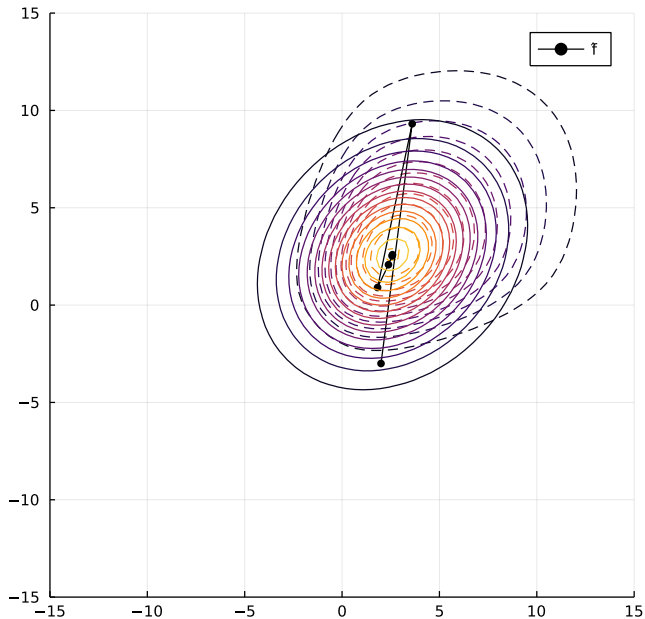
$$p(f | y) \approx \mathcal{N}(f | \hat{f}, -(\mathrm{d}^2 \log h / \mathrm{d}f^2)^{-1})$$



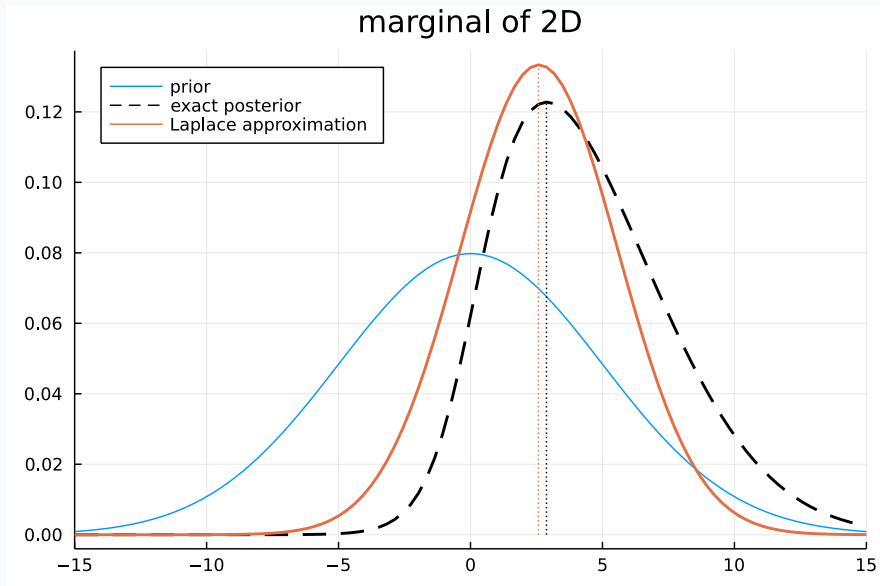
$$p(f | y) \approx \mathcal{N}(f | \hat{f}, -(\mathrm{d}^2 \log h / \mathrm{d}f^2)^{-1}) = q(f)$$



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 $q(\mathbf{f})$

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

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

$$D_{\text{KL}}(p\|q) = \text{KL}[p(x)\|q(x)] = \mathbb{E}_{x \sim p} \left[\log \frac{p(x)}{q(x)} \right] = \int p(x) \left[\log \frac{p(x)}{q(x)} \right] dx$$

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

Demo: KL between two Gaussians

tinyurl.com/nongaussian-inference-viz-v1

Minimising divergences

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

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

Expectation Propagation (EP)

Expectation Propagation

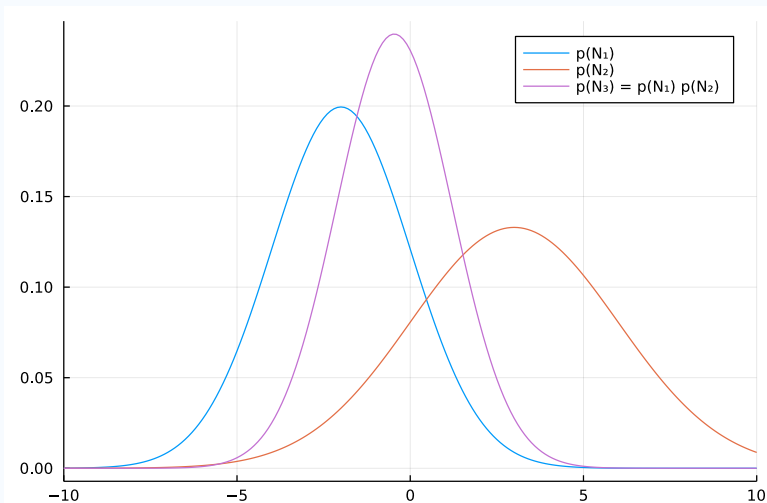
Exact posterior:

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

Approximate posterior:

$$q(\mathbf{f}) \propto p(\mathbf{f}) \prod_{i=1}^N t_i(f_i)$$
$$t_i = Z_i \mathcal{N}(f_i | \tilde{\mu}_i, \tilde{\sigma}_i^2)$$

Multiplying and dividing Gaussians



Adding and subtracting natural (canonical) parameters

Expectation Propagation iterations

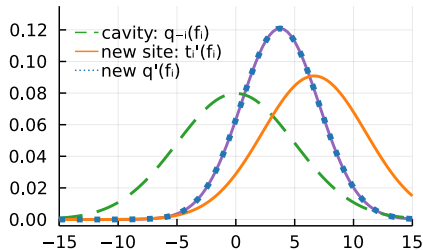
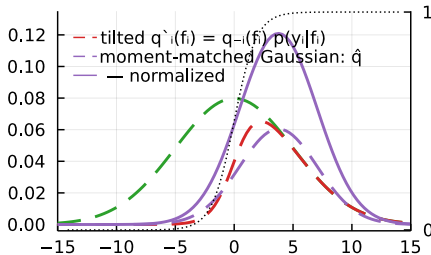
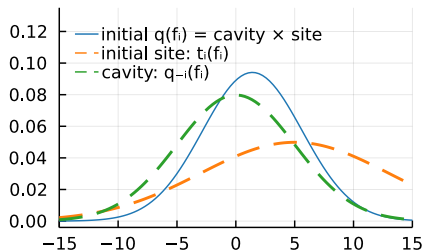
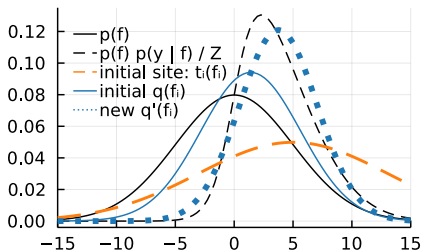
$$\text{"min KL}[p(\mathbf{f} | \mathbf{y}) \| q(\mathbf{f})]" \qquad q(\mathbf{f}) \propto p(\mathbf{f}) \prod_{i=1}^N \underbrace{t_i(f_i)}_{\text{site} \propto \mathcal{N}(f_i)}$$

For each site i :

1. marginalize $\int q(\mathbf{f}) \, df_{j \neq i} = q(f_i) \not\propto t_i(f_i)$
2. improve local approximation: $\min \text{KL}[q(f_i) \frac{p(y_i | f_i)}{t_i(f_i)} \| q(f_i) \frac{t'_i(f_i)}{t_i(f_i)}]$
 - 2.1 cavity distribution $q_{-i}(f_i) = \frac{q(f_i)}{t_i(f_i)} \Leftrightarrow q(f_i) = q_{-i}(f_i) t_i(f_i)$
 - 2.2 tilted distribution $q_{\setminus i}(f_i) = q_{-i}(f_i) p(y_i | f_i)$
 - 2.3 argmin $\text{KL}[q_{-i}(f_i) p(y_i | f_i) \| \hat{q}]$ by moment-matching
 - 2.4 update site: $t'_i(f_i) = \frac{\hat{q}}{q_{-i}(f_i)} \Leftrightarrow \hat{q} = q_{-i}(f_i) t'_i(f_i)$
3. compute new $q'(\mathbf{f})$ (rank-1 update)

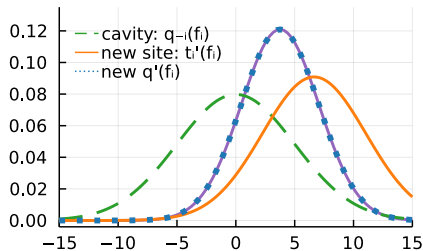
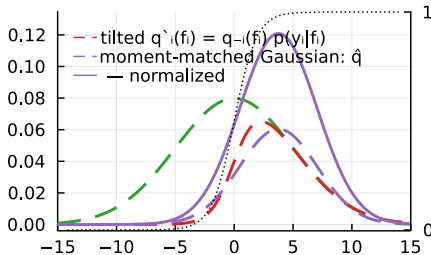
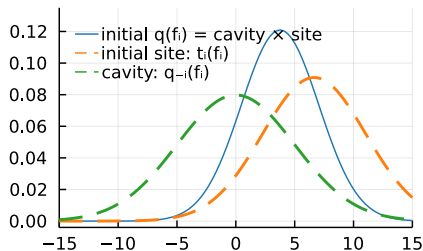
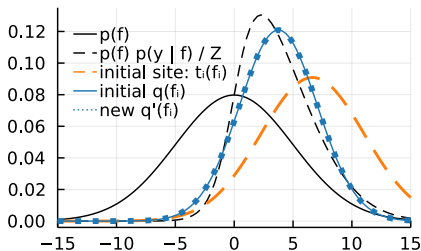
Expectation Propagation in 1D

iteration 1



Expectation Propagation in 1D

iteration 2

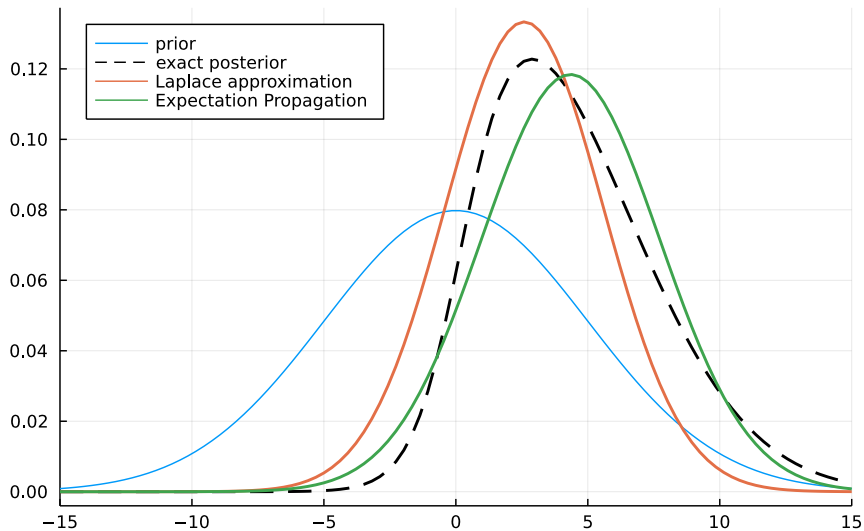


Demo: EP in 2D

tinyurl.com/nongaussian-inference-viz-v1

Marginals

marginal of 2D



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

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

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

Variational Bayes (VB)

Variational Inference (VI)

Variational Bayes (VB)

Idea:

minimise divergence between $p(f | y)$ and $q(f)$ the “other” way

$$\operatorname{argmin}_{\mu, \Sigma} \text{KL} [q(f) \| p(f | y)]$$

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

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

$$\begin{aligned}\log p(y) &= \int q(f) [\log p(y|f)] df - \text{KL}[q(f) \| p(f)] + \text{KL}[q(f) \| p(f|y)] \\ &\geq \int q(f) [\log p(y|f)] df - \text{KL}[q(f) \| p(f)]\end{aligned}$$

Lower bound on the (log-)evidence $p(y) = \text{ELBO}$

Likelihood term

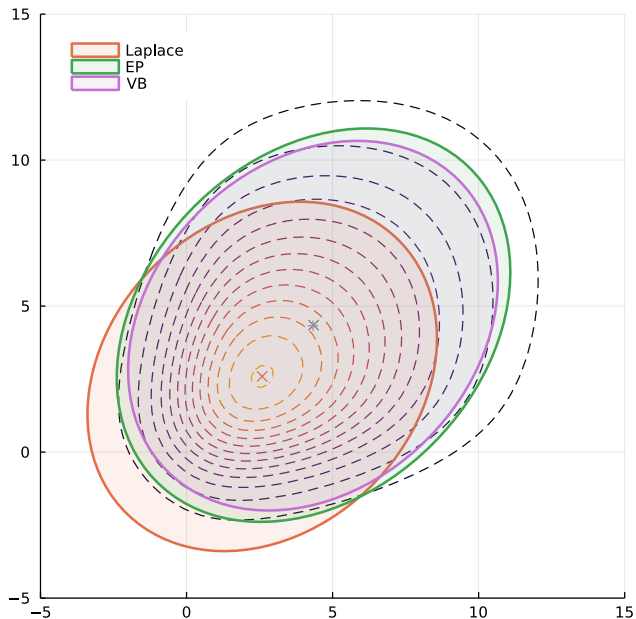
Integral separates for a factorizing likelihood:

$$\begin{aligned} & \int q(\mathbf{f}) [\log p(\mathbf{y} | \mathbf{f})] d\mathbf{f} \\ &= \sum_{i=1}^N \int q(f_i) [\log p(y_i | f_i)] df_i \end{aligned}$$

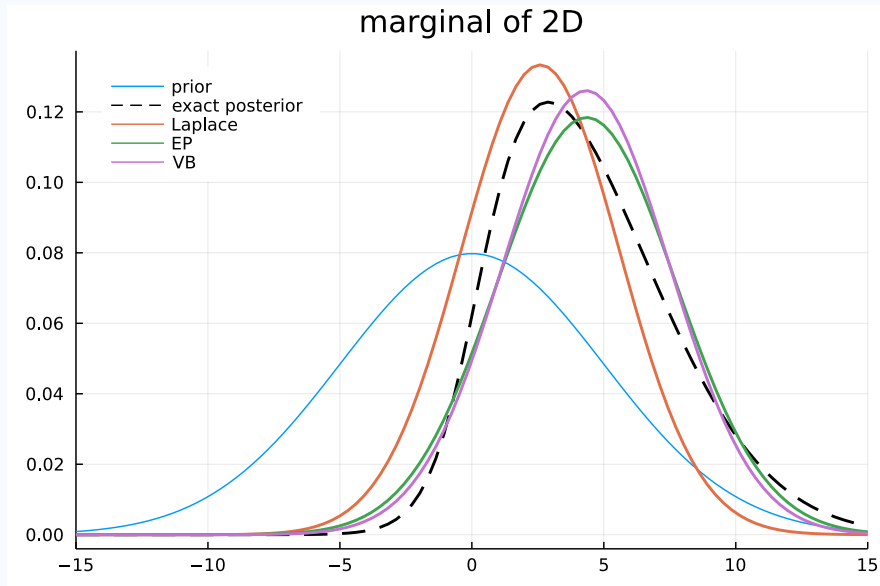
Evaluating the 1D integrals:

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

Comparison 2D



Marginals



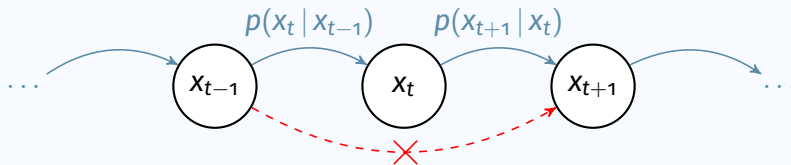
Variational Bayes: important properties

- principled: directly minimising divergence from true posterior
- mode-seeking (e.g. multi-modal posterior: fits just one)
 - + minimises a true lower bound \rightarrow convergence
 - underestimates variance

- ✓ 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. Comparison

Markov Chain Monte Carlo

Markov Chain



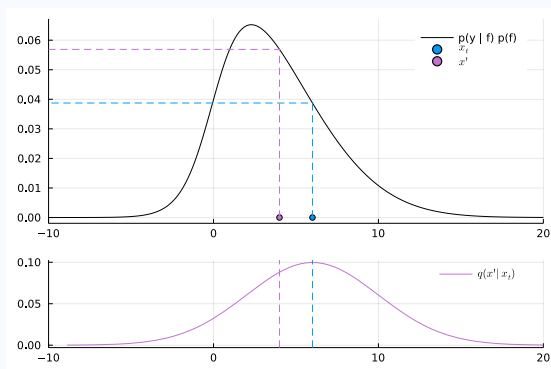
- Samples x_1, \dots, x_T
- “Markov” = 1-step history
- $x_{t+1} \sim p(x_{t+1} | x_t)$, independent of x_{t-1}, \dots, x_1

Markov Chain Monte Carlo (MCMC)

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

Requires:

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



In each iteration t :

1. Random proposal $x' \sim q(x' | x_t)$
2. Acceptance probability $\frac{h(x')}{h(x_t)} \rightarrow$ ensures sampling from $p(f | y)$

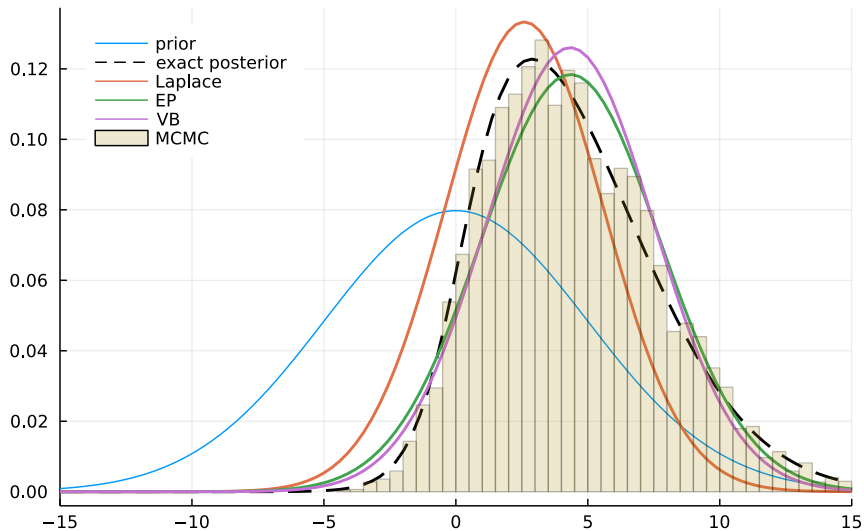
accept: $x_{t+1} = x'$ reject: copy $x_{t+1} = x_t$

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

Demo: MCMC in 2D

tinyurl.com/nongaussian-inference-viz-v1

marginal of 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) → use robust implementations
 - + 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



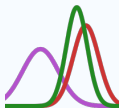
PyMC3

■ TensorFlow Probability (GPflow)



GPflow

■ Turing.jl



- ✓ Gaussian processes with Gaussian likelihood
- ✓ What is the likelihood? Connecting observations and Gaussian process prior
- ✓ Non-Gaussian likelihoods: what happens to the posterior?
- ✓ How to approximate the intractable
 - ✓ with Gaussians
 - Laplace
 - Expectation Propagation
 - Variational Bayes
 - ✓ with samples: MCMC

5. Comparison

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 $\text{KL}[q(f) \| p(f | y)]$
- ▶ principled, any likelihood
- ▶ underestimates variance

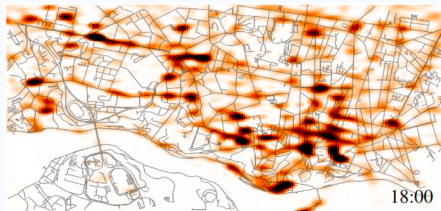
What we did not cover...

- More complex likelihoods (heteroskedastic, zero-inflated, multi-stage...)
- Marginal likelihood approximations for hyperparameter learning [7]
- How parametrisation affects Gaussianity of $p(f | y)$
- Connections between EP and VB (“PowerEP”) [1]
- Combinations of MCMC and variational methods
- Augmenting likelihood with auxiliary variable
→ conditionally conjugate model [2]

Take-away

We can...

- create **richer models** with likelihoods beyond the Gaussian
- **learn latent functions** that form the connection between data points
- handle the non-Gaussian posterior with **approximations**
- **trade off** speed, accuracy, and ease-of-use



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