

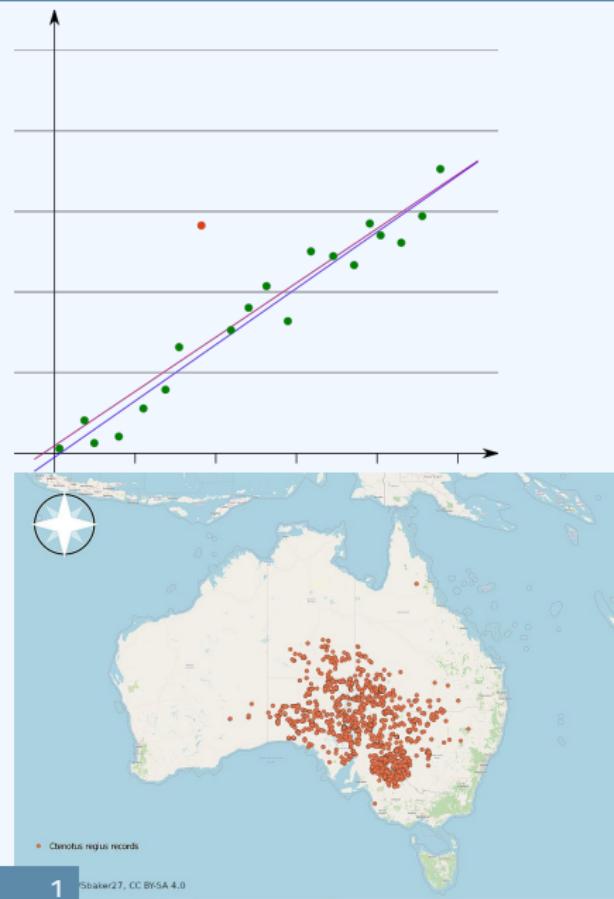
GAUSSIAN PROCESSES FOR NON-GAUSSIAN LIKELIHOODS

ST JOHN

Finnish Center for Artificial Intelligence
& Aalto University

GAUSSIAN PROCESS SUMMER SCHOOL, 14 SEPTEMBER 2021

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. Comparisons

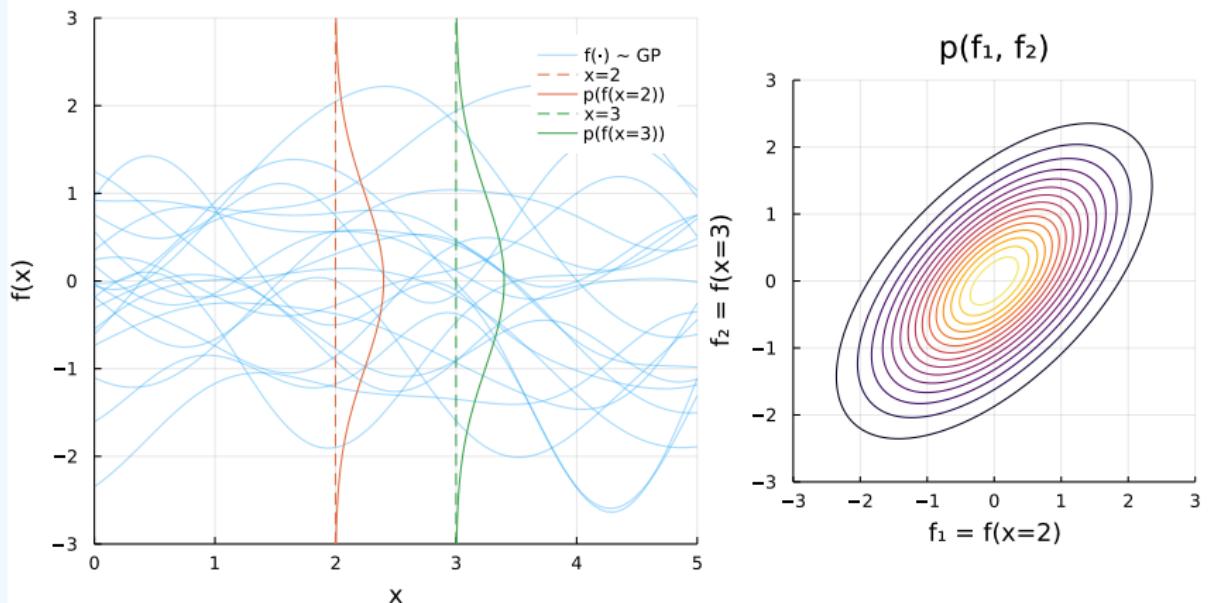
- | | |
|----------------------------------|----------------------|
| + <i>Intuitive</i> understanding | - In-depth expertise |
| + Learning the language | - Lots of maths |

SETTING THE SCENE

GAUSSIAN PROCESS $f(\cdot)$

Distribution over *functions*

Marginals are Gaussian (mean and covariance)

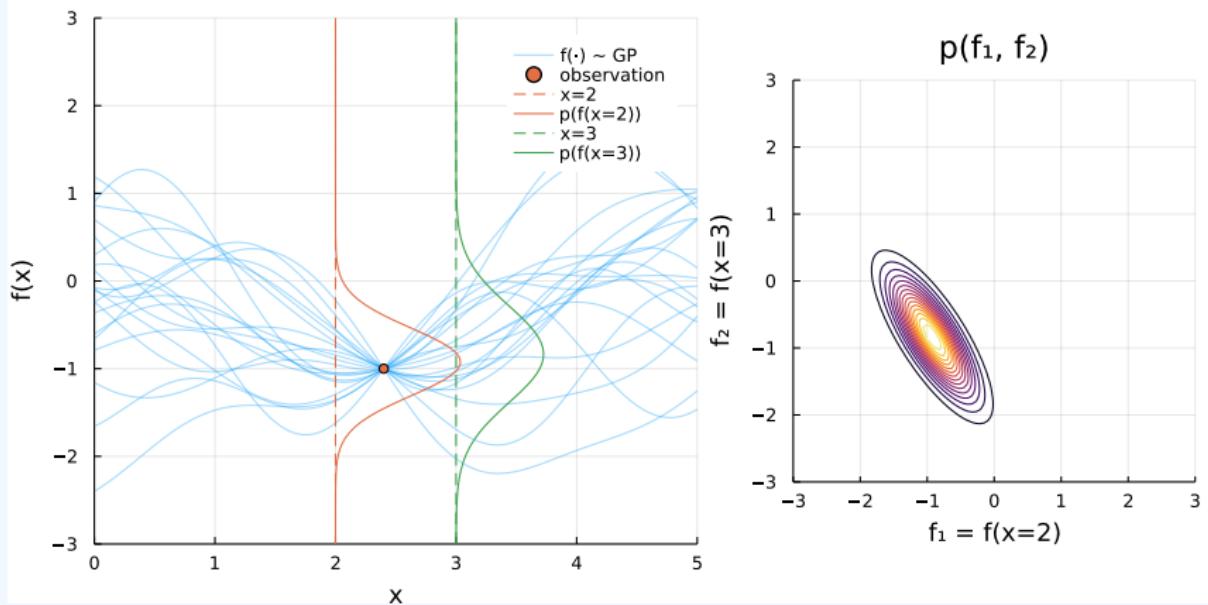


infinitecuriosity.org/vizgp

GAUSSIAN PROCESS CONDITIONED ON OBSERVATION

Distribution over *functions*

Marginals are Gaussian (mean and covariance)

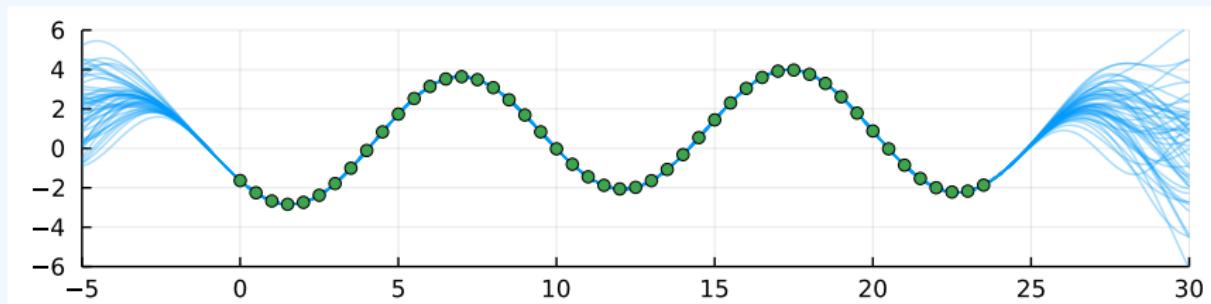


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GAUSSIAN NOISE MODEL

Without noise model, we interpolate observations:

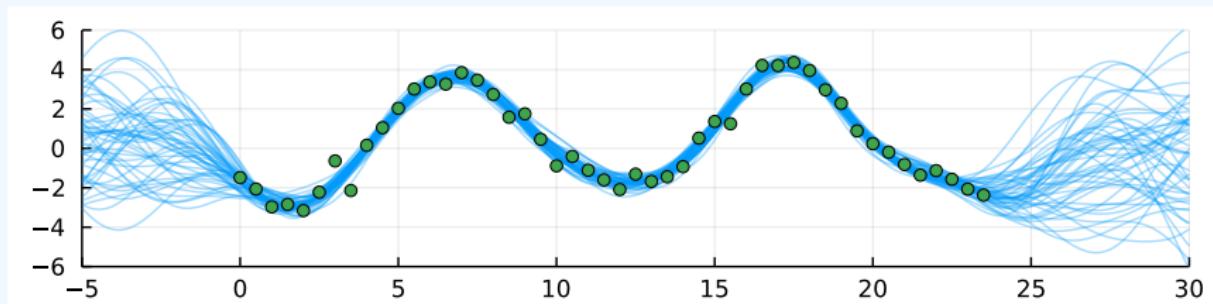
$$y(x) = f(x) + \epsilon \quad \epsilon \stackrel{\text{indep}}{\sim} \mathcal{N}(0, \sigma_{\text{noise}}^2)$$
$$\text{or } f = \mathcal{N}(y|f, \sigma_{\text{noise}}^2)$$



GAUSSIAN NOISE MODEL

Gaussian additive noise model, written two ways:

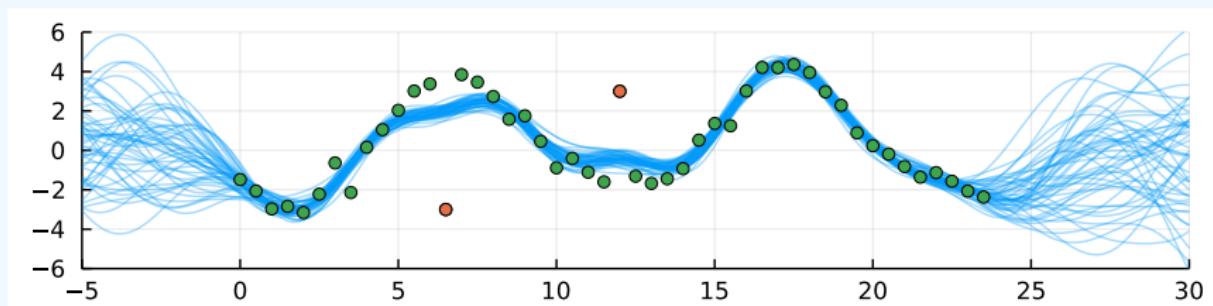
$$y(x) = f(x) + \epsilon, \quad \epsilon \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_{\text{noise}}^2)$$
$$p(y | f) = \mathcal{N}(y | f, \sigma_{\text{noise}}^2)$$



MISSPECIFIED GAUSSIAN NOISE MODEL

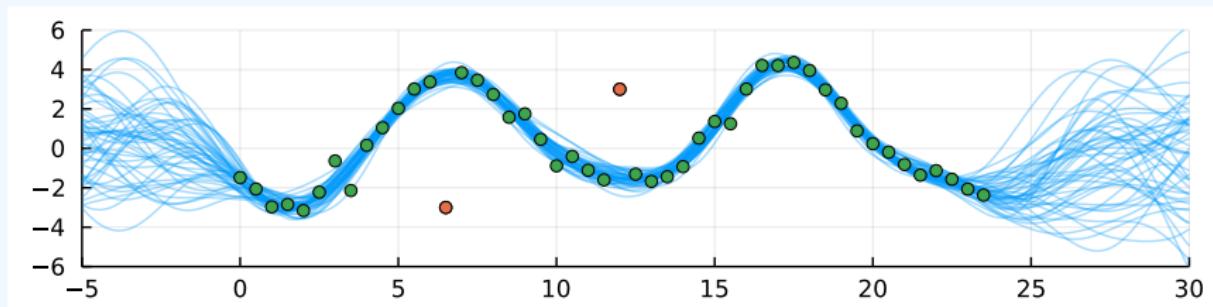
Gaussian additive noise model, written two ways:

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



HEAVY-TAILED NOISE MODEL

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



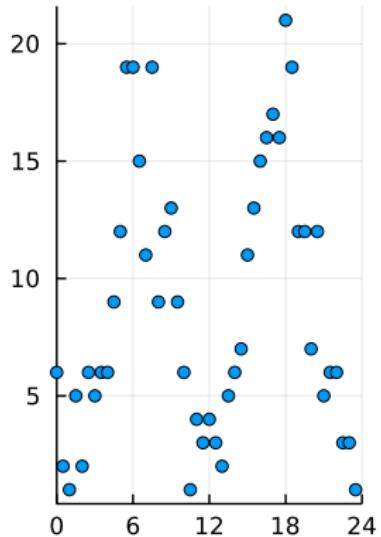
OUTLINE

- ✓ 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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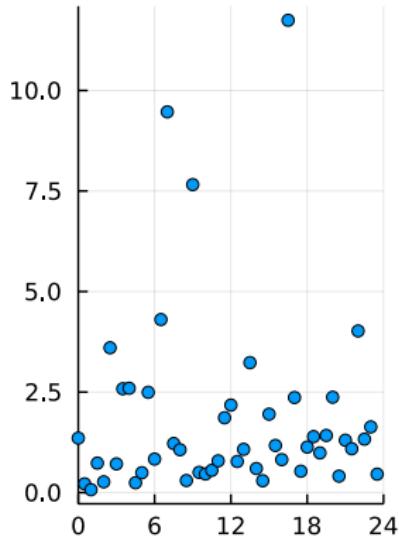
LIKELIHOOD

NON-GAUSSIAN OBSERVATIONS

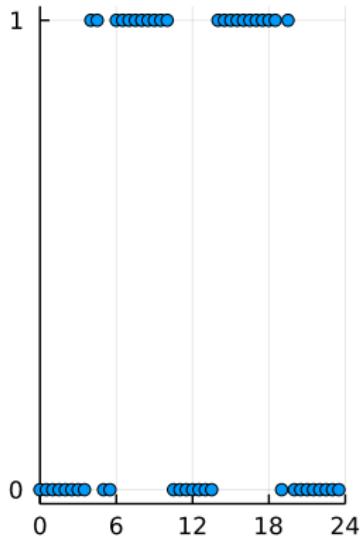
Case count



Rainfall



Awake: y/n?



latent functional relationship

Likelihood

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

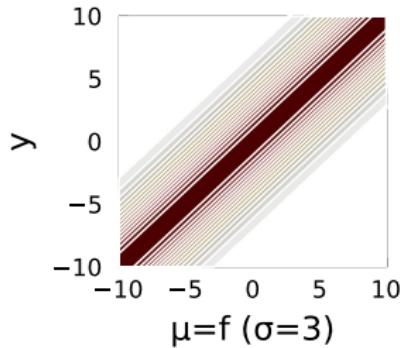
factorizing

$$p(y \mid f)$$

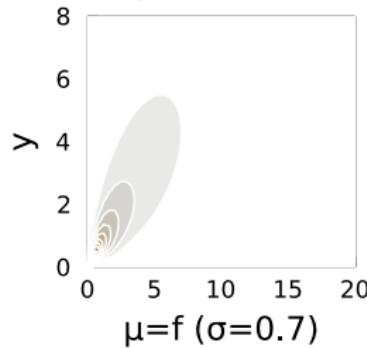
Function of two arguments:
 $y \mapsto p(y \mid f), \quad f \mapsto p(y \mid f)$

$$p(y | f)$$

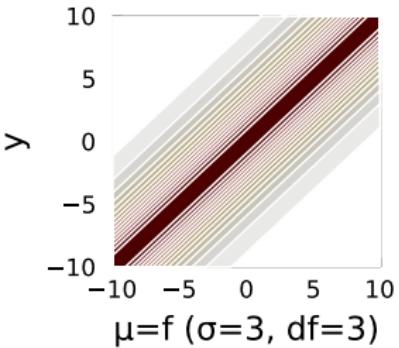
Gaussian



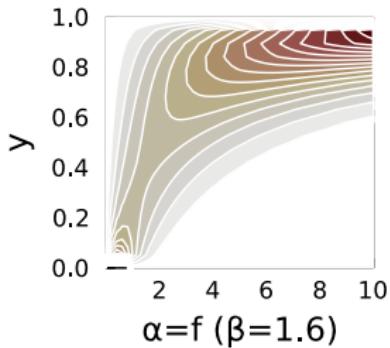
Log-Gaussian



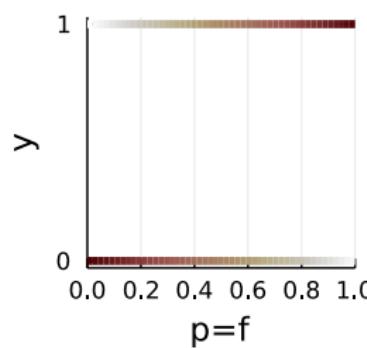
Student's t



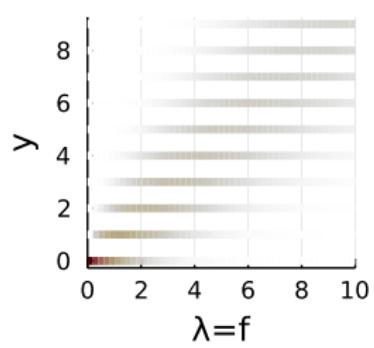
Beta



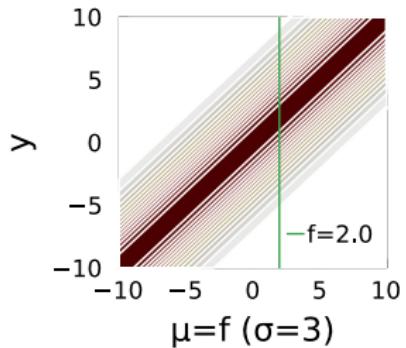
Bernoulli



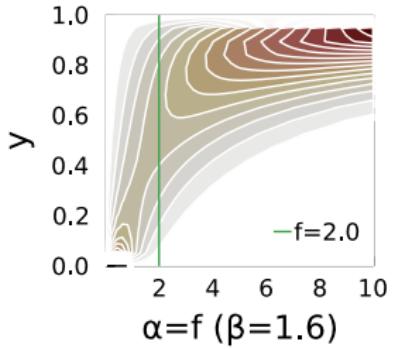
Poisson



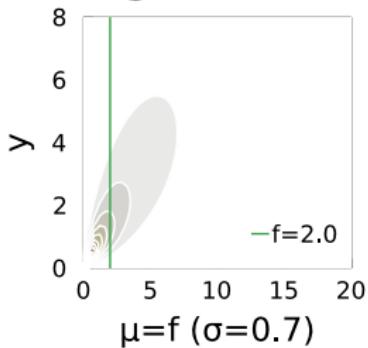
Gaussian



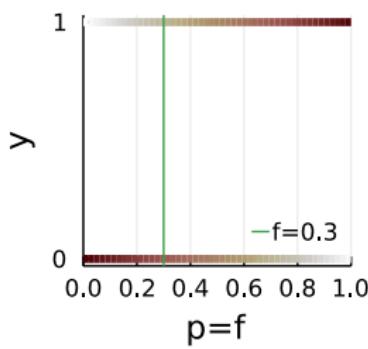
Beta



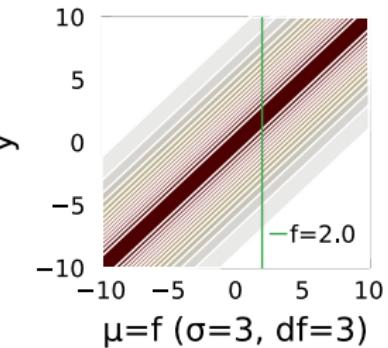
Log-Gaussian



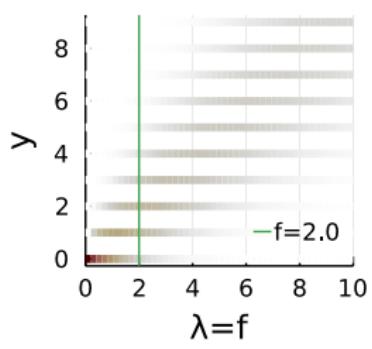
Bernoulli



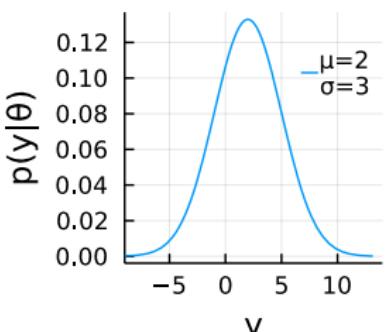
Student's t



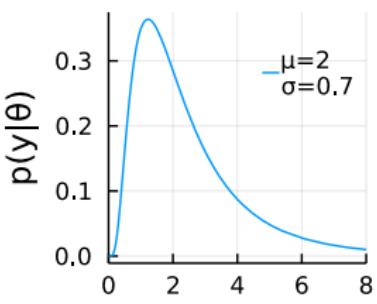
Poisson



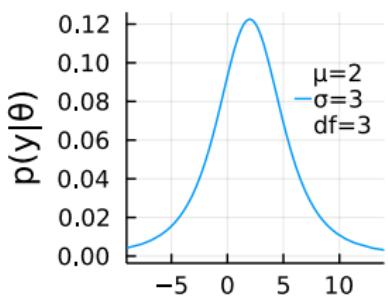
Gaussian



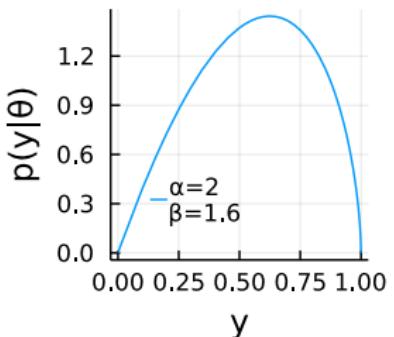
Log-Gaussian



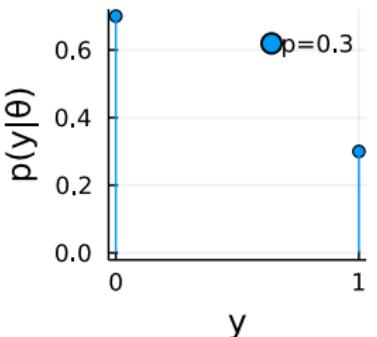
Student's t



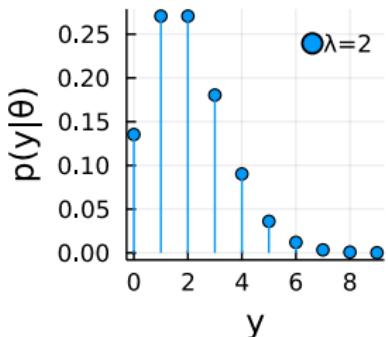
Beta



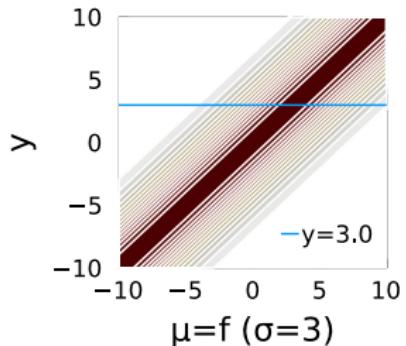
Bernoulli



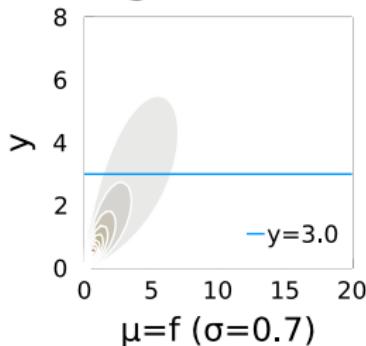
Poisson



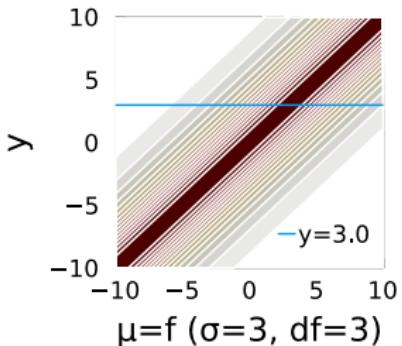
Gaussian

 $\mu=f (\sigma=3)$

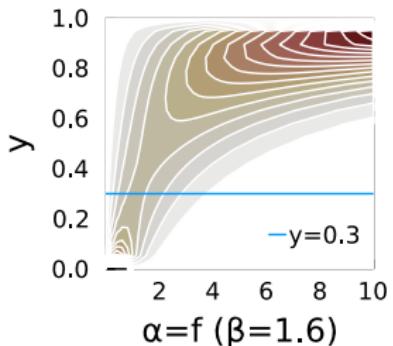
Log-Gaussian

 $\mu=f (\sigma=0.7)$

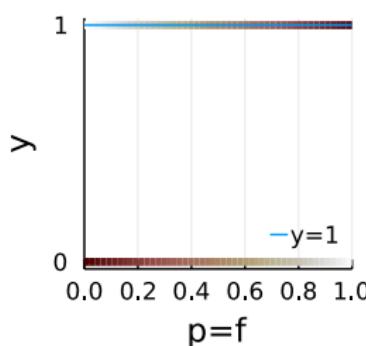
Student's t

 $\mu=f (\sigma=3, df=3)$

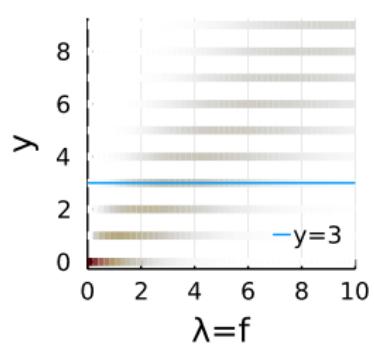
Beta

 $\alpha=f (\beta=1.6)$

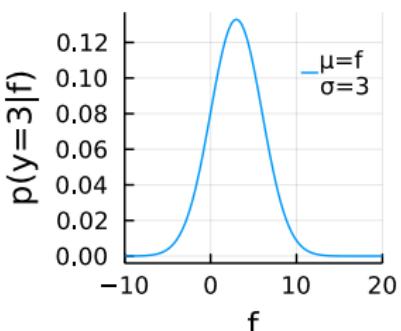
Bernoulli

 $p=f$

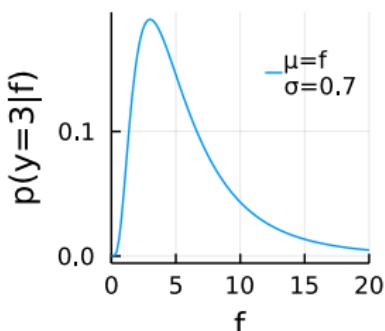
Poisson

 $\lambda=f$

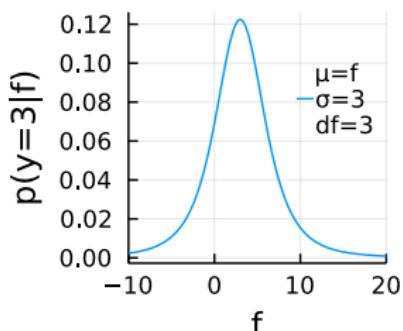
Gaussian



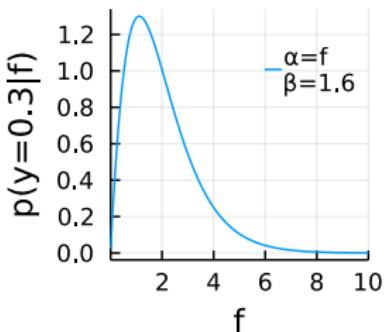
Log-Gaussian



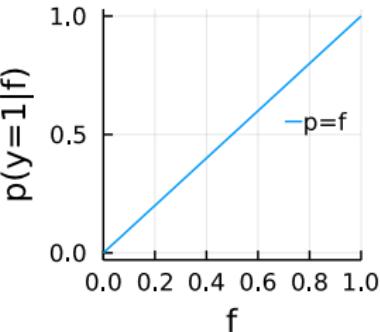
Student's t



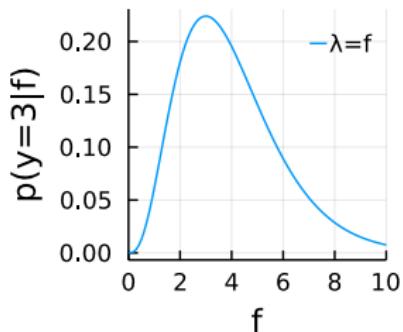
Beta



Bernoulli



Poisson



Two aspects of likelihoods:

1. link functions
2. log-concavity

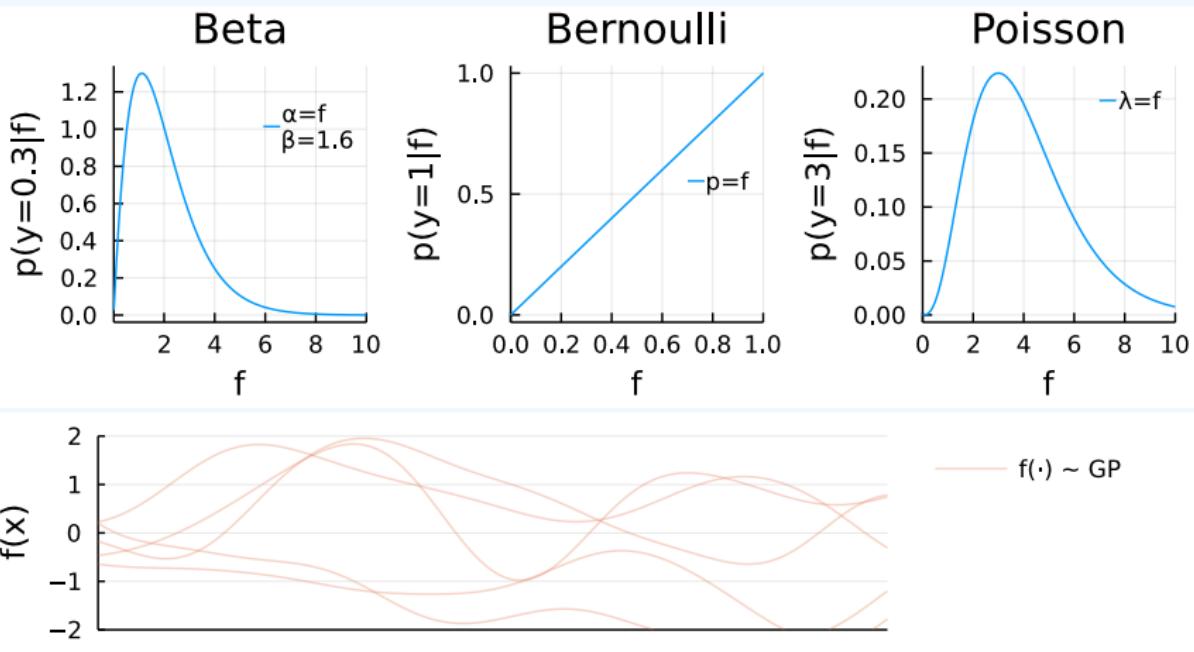
LINK FUNCTIONS

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

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

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

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



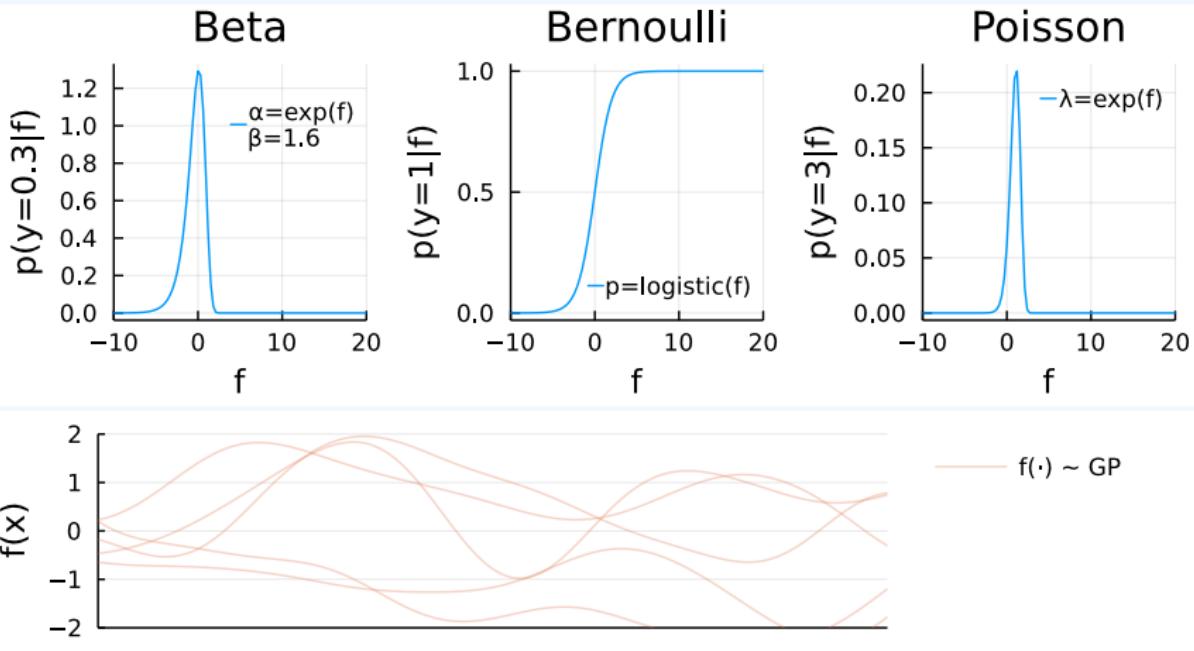
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LINK FUNCTIONS

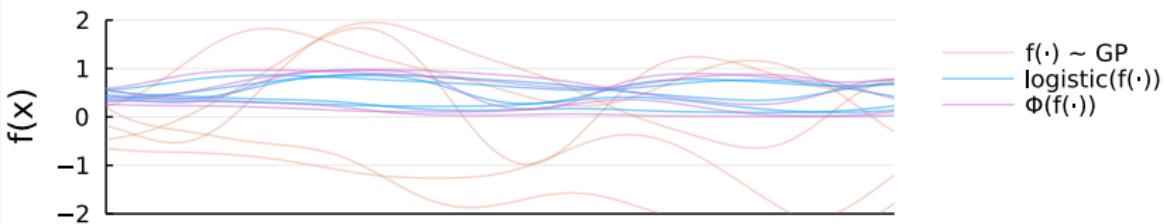
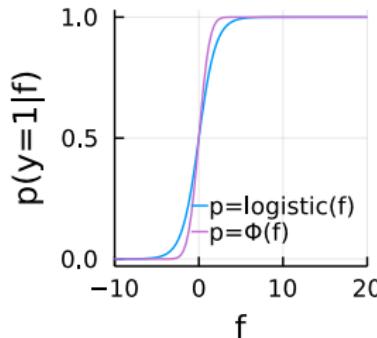
$$\mathbb{E}[y] = \theta \in (0 \dots \infty)$$

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

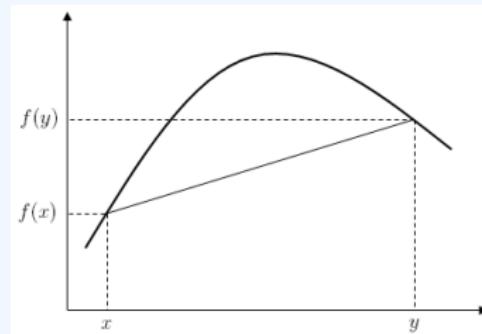
$$\text{link}(\theta) = f$$

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

Bernoulli



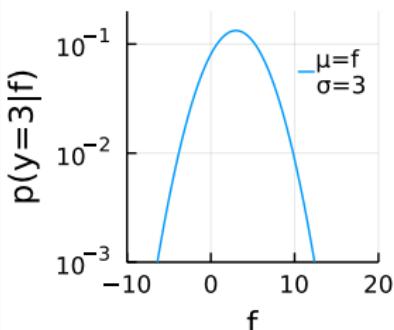
(LOG-)CONCAVITY



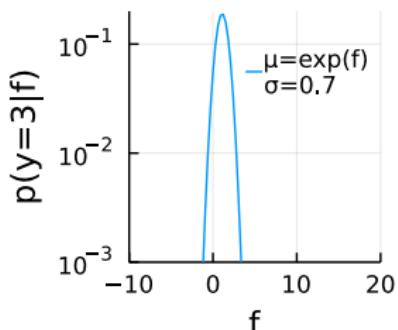
$$f(\alpha x + (1 - \alpha)y) \geq \alpha f(x) + (1 - \alpha)f(y)$$

LOG-CONCAVITY OF LIKELIHOODS

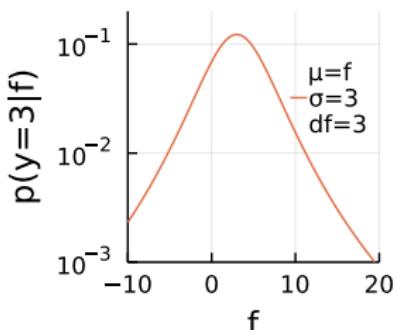
Gaussian



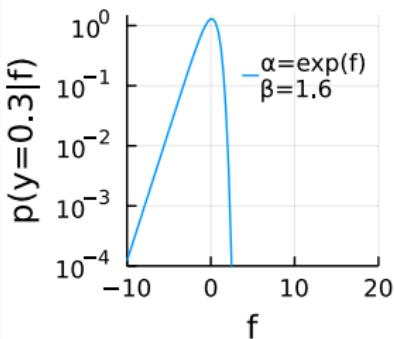
Log-Gaussian



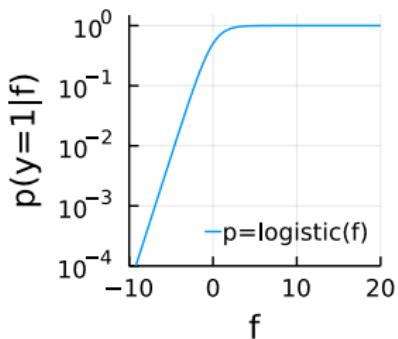
Student's t



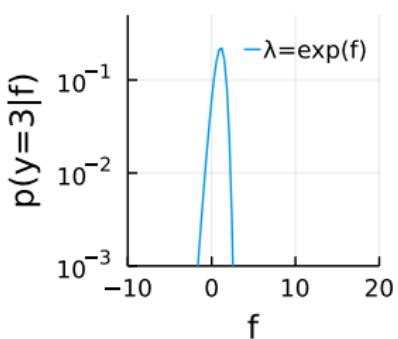
Beta



Bernoulli



Poisson



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- ✓ Gaussian processes with Gaussian likelihood
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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}**

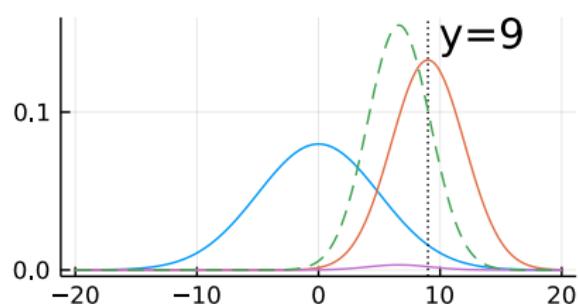
$$p(\mathbf{f} \mid \mathbf{y}) = \frac{1}{Z} p(\mathbf{f}) \prod_{i=1}^N p(y_i \mid f_i)$$

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

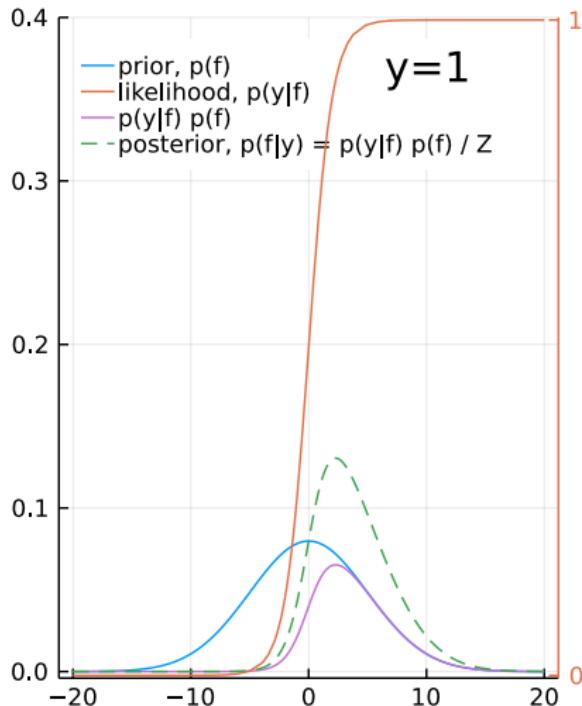
- & Gaussian likelihood: conjugate case \rightarrow posterior Gaussian
- & non-Gaussian $p(y|f) \rightarrow p(\mathbf{f} \mid \mathbf{y})$ also non-Gaussian, intractable

1D EXAMPLES

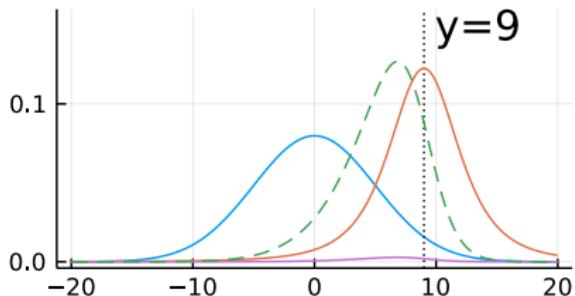
Gaussian



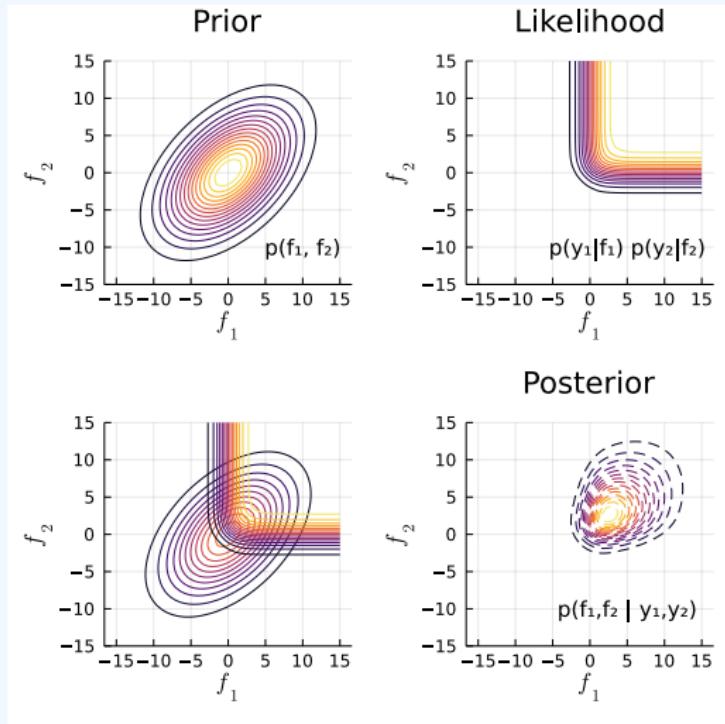
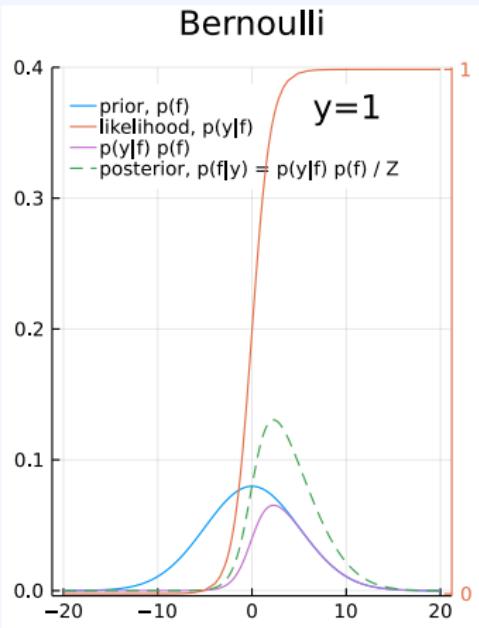
Bernoulli



Student's t



BERNOULLI EXAMPLE IN 2D



POSTERIOR FOR N OBSERVATIONS

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

$$f_1 = f(x_1)$$

$$f_2 = f(x_2)$$

⋮

$$f_N = f(x_N)$$

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?! :)

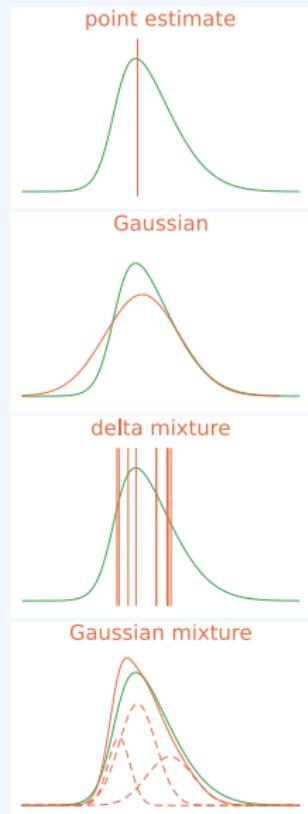
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APPROXIMATIONS

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 $q(\mathbf{f})$

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

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

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

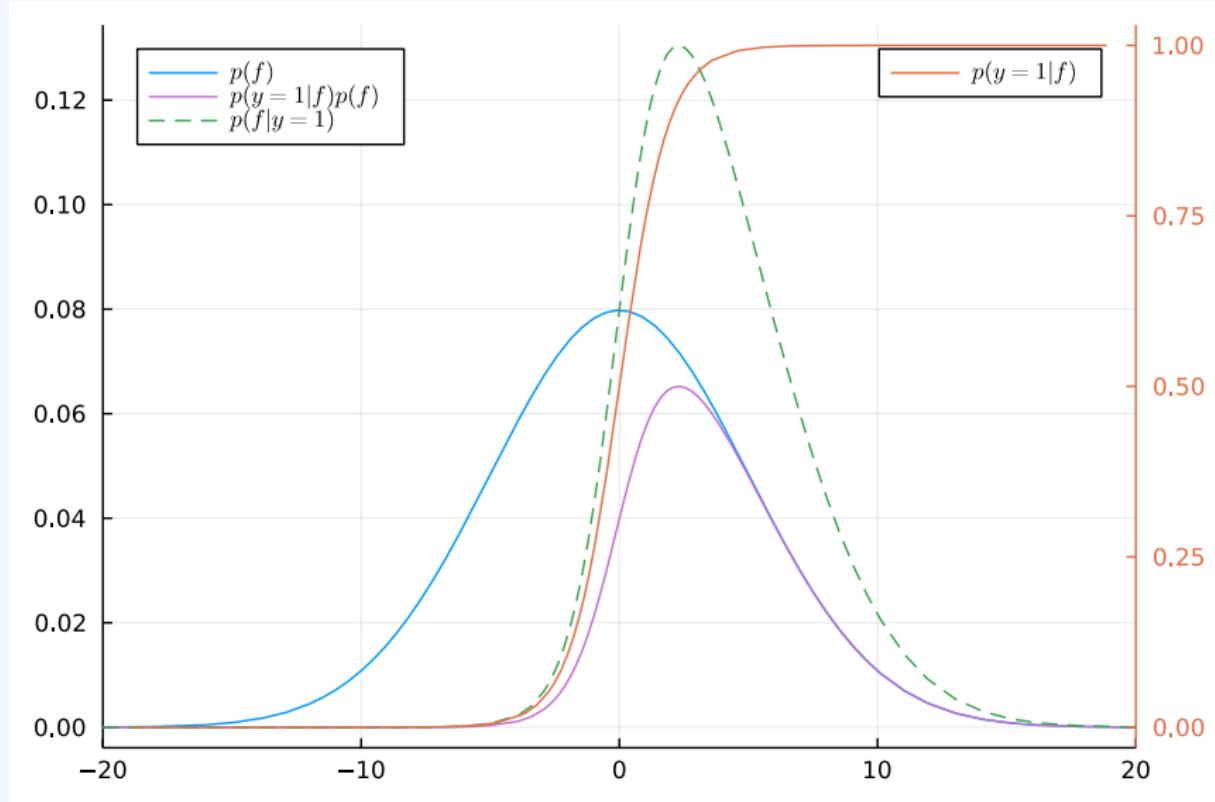
Approximate quadratic polynomial:

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

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

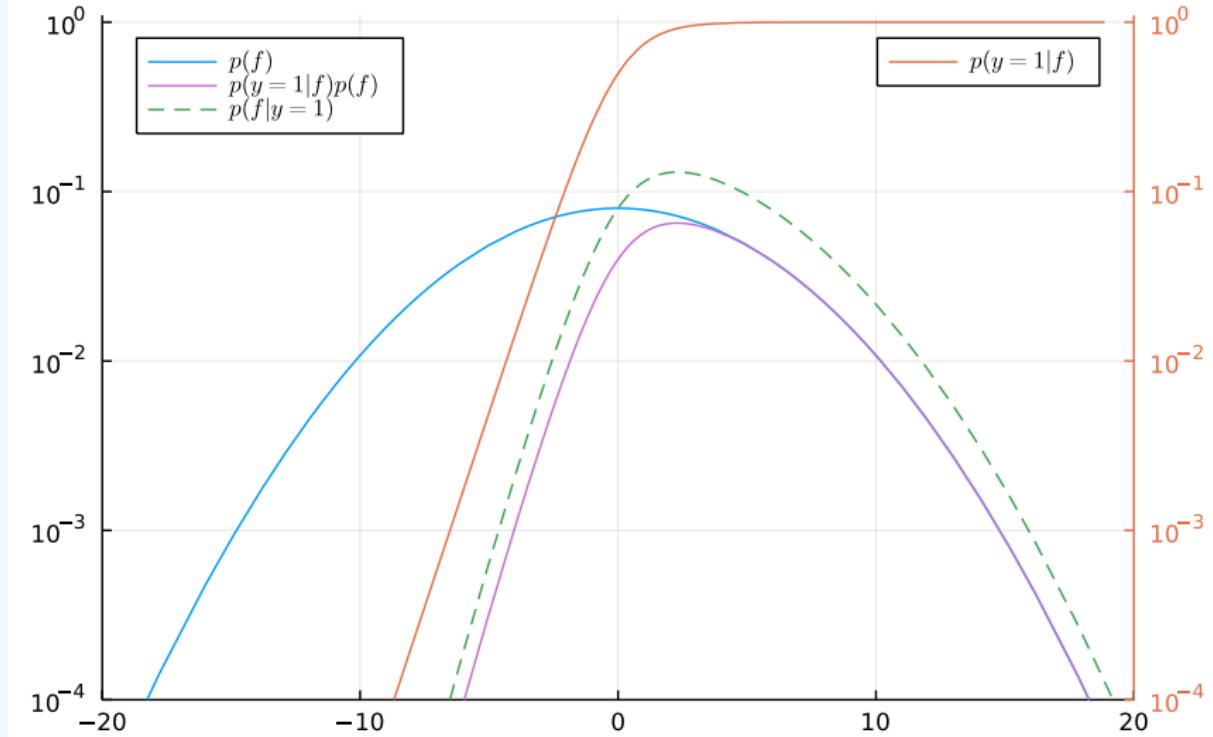
1. Find mode of posterior
2nd-order gradient optimisation (e.g. Newton's method)
2. Match curvature (Hessian) at mode

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

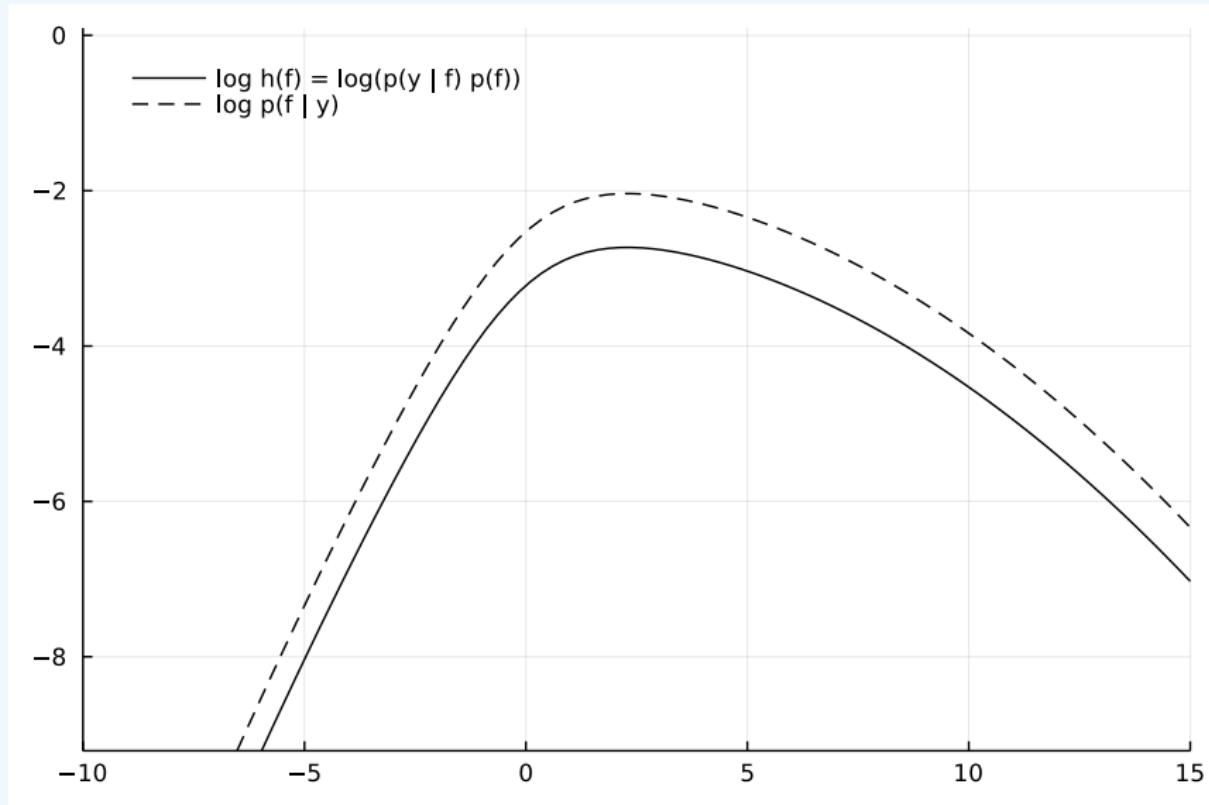


$$\log p(f | y) = -\log Z + \log p(y | f) + \log p(f)$$

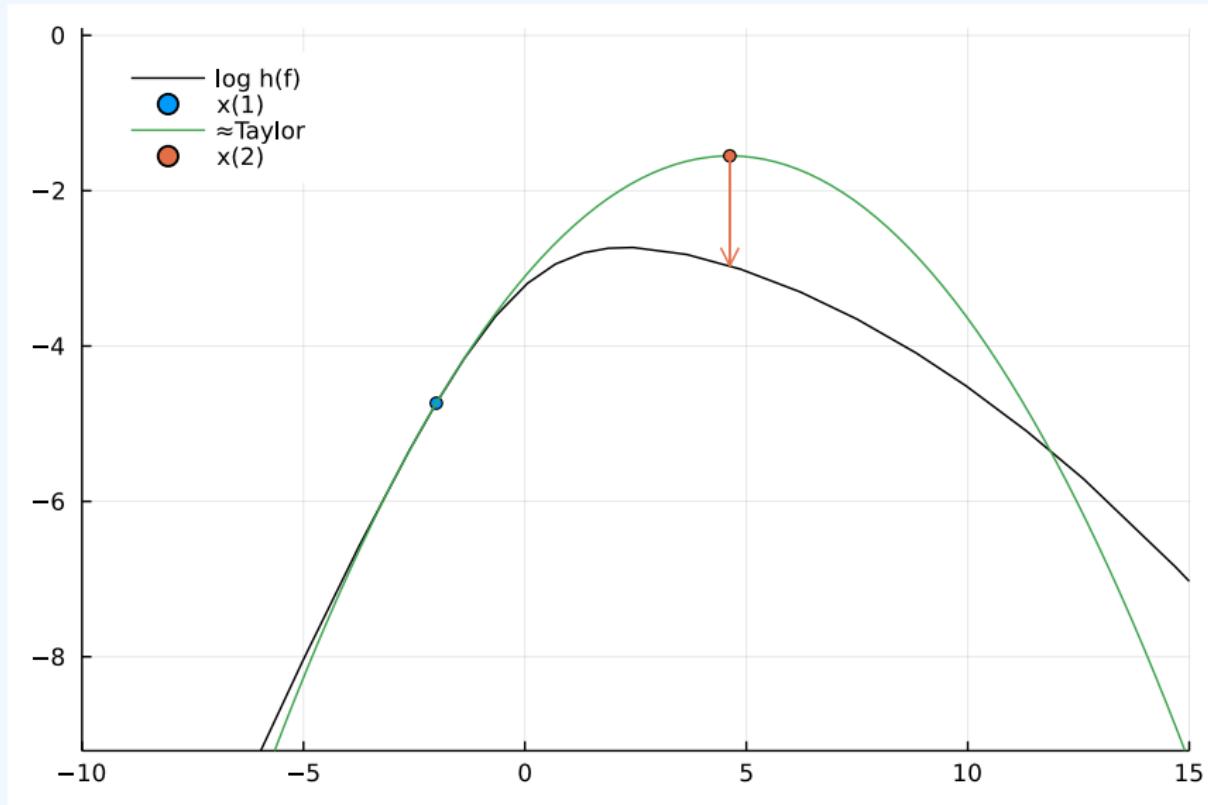
log scale



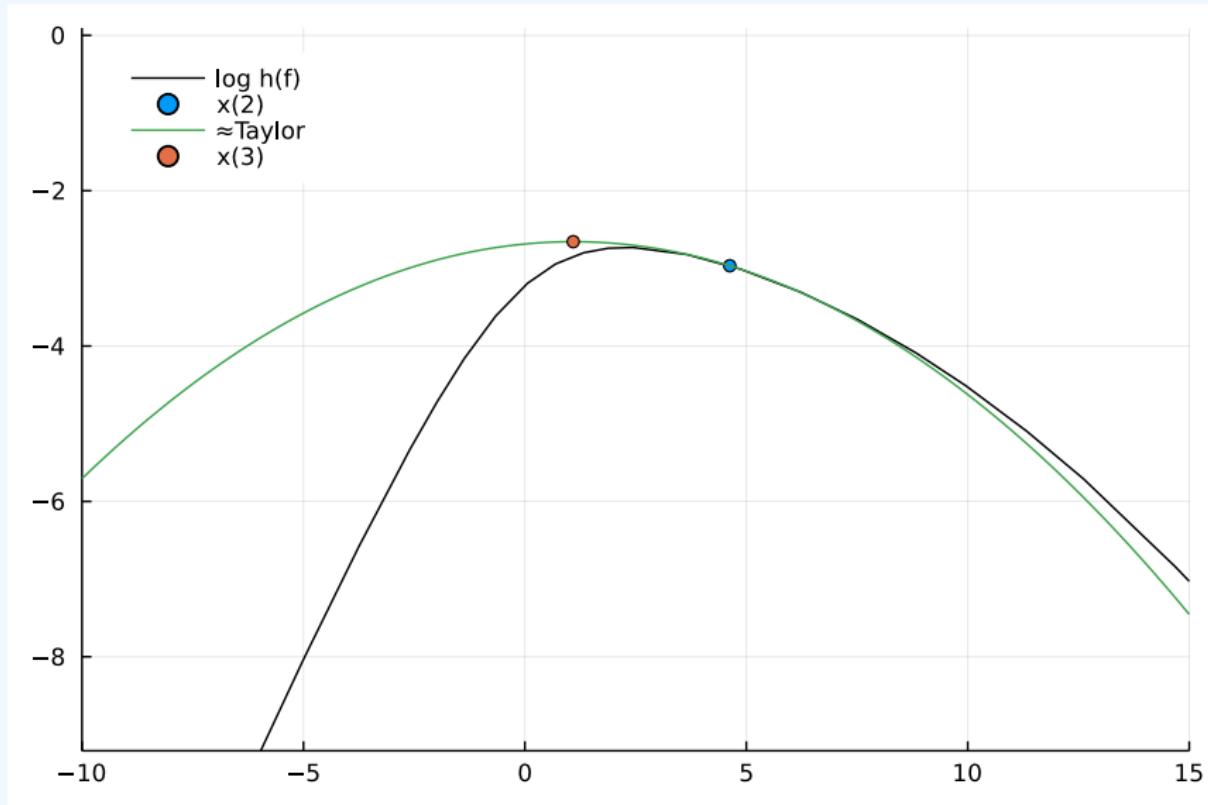
$$\log p(f \mid y) = -\log Z + \log h(f)$$



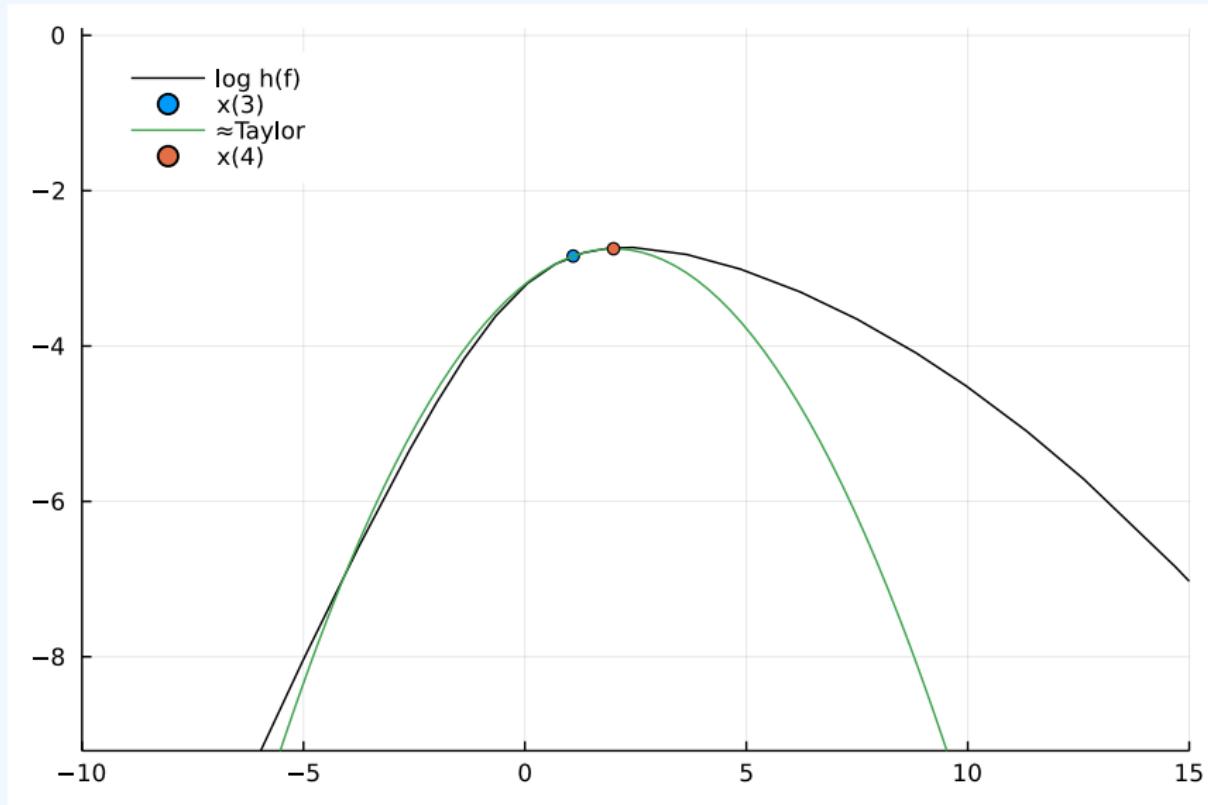
NEWTON'S METHOD



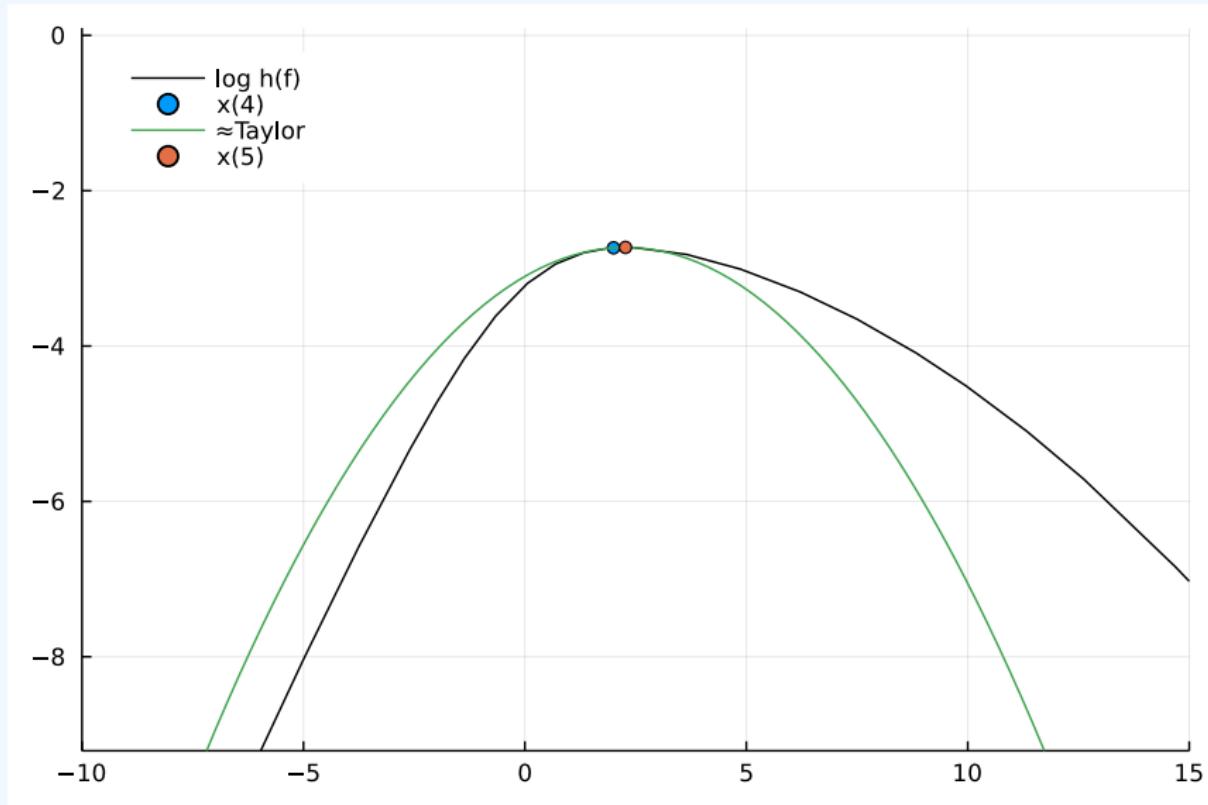
NEWTON'S METHOD



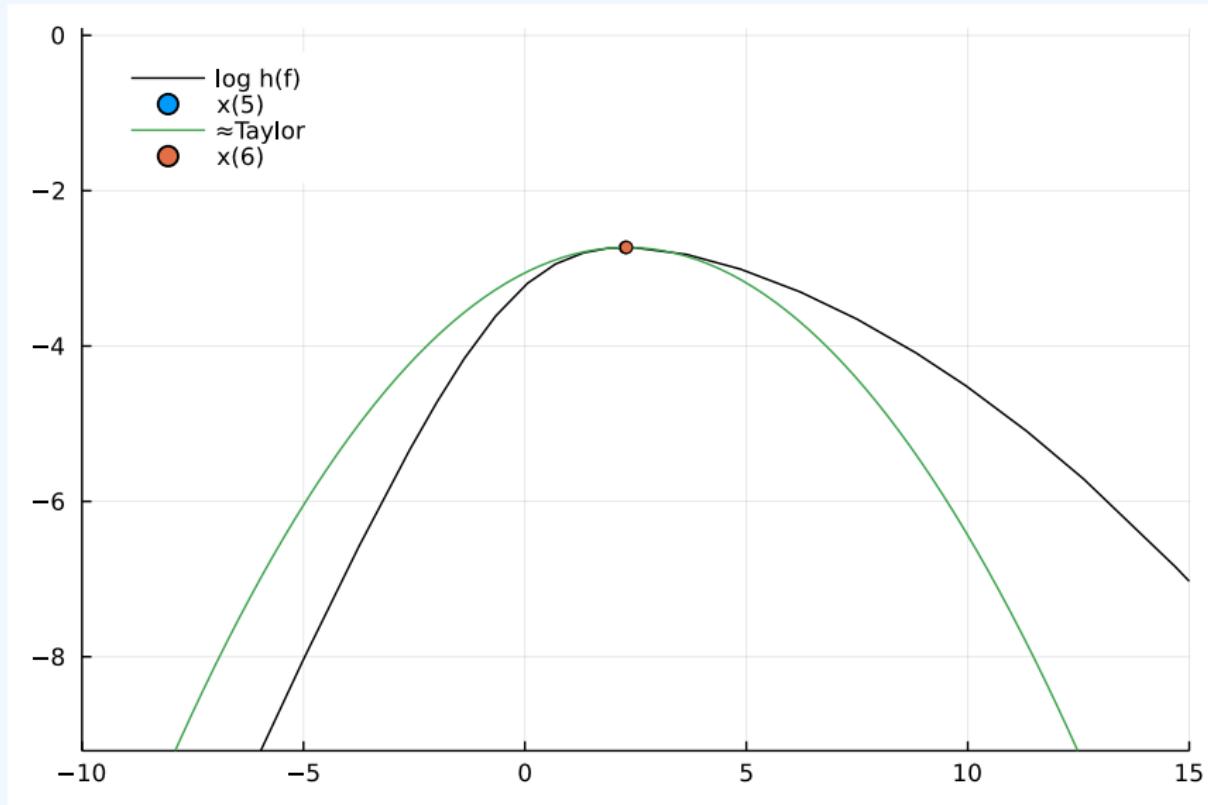
NEWTON'S METHOD



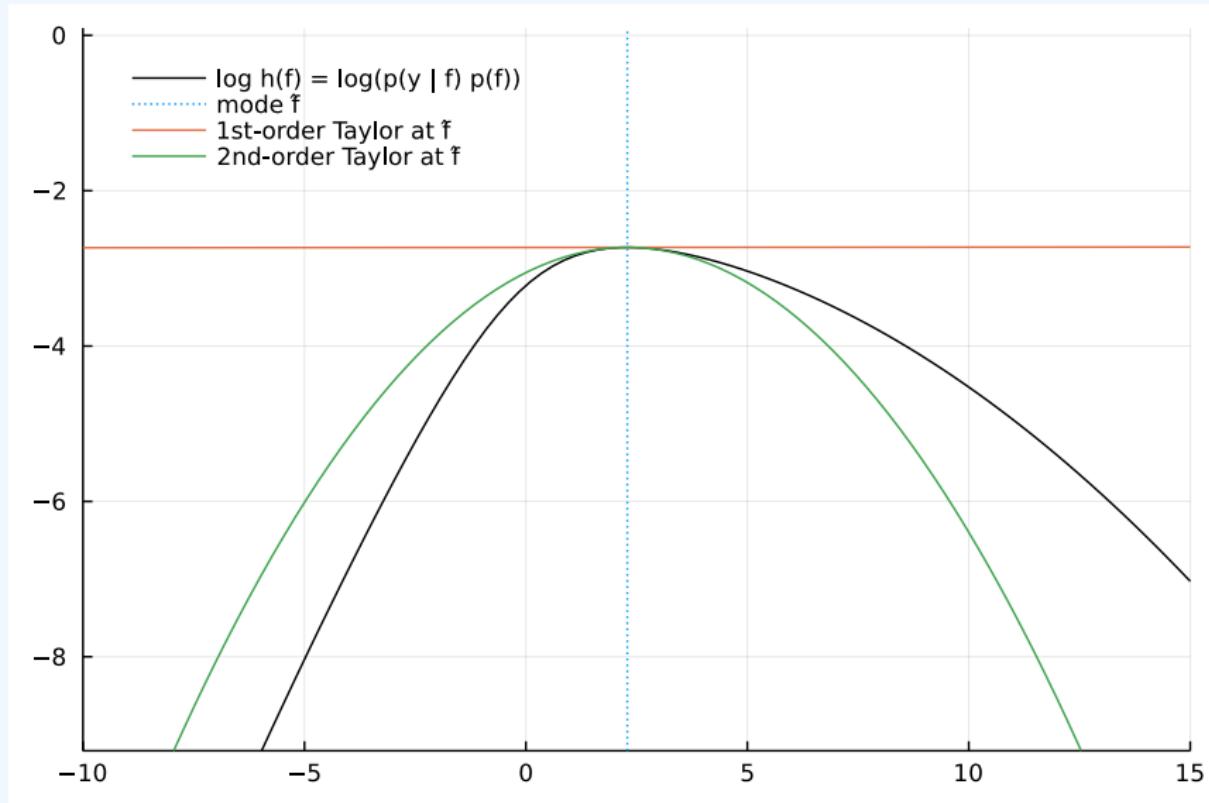
NEWTON'S METHOD



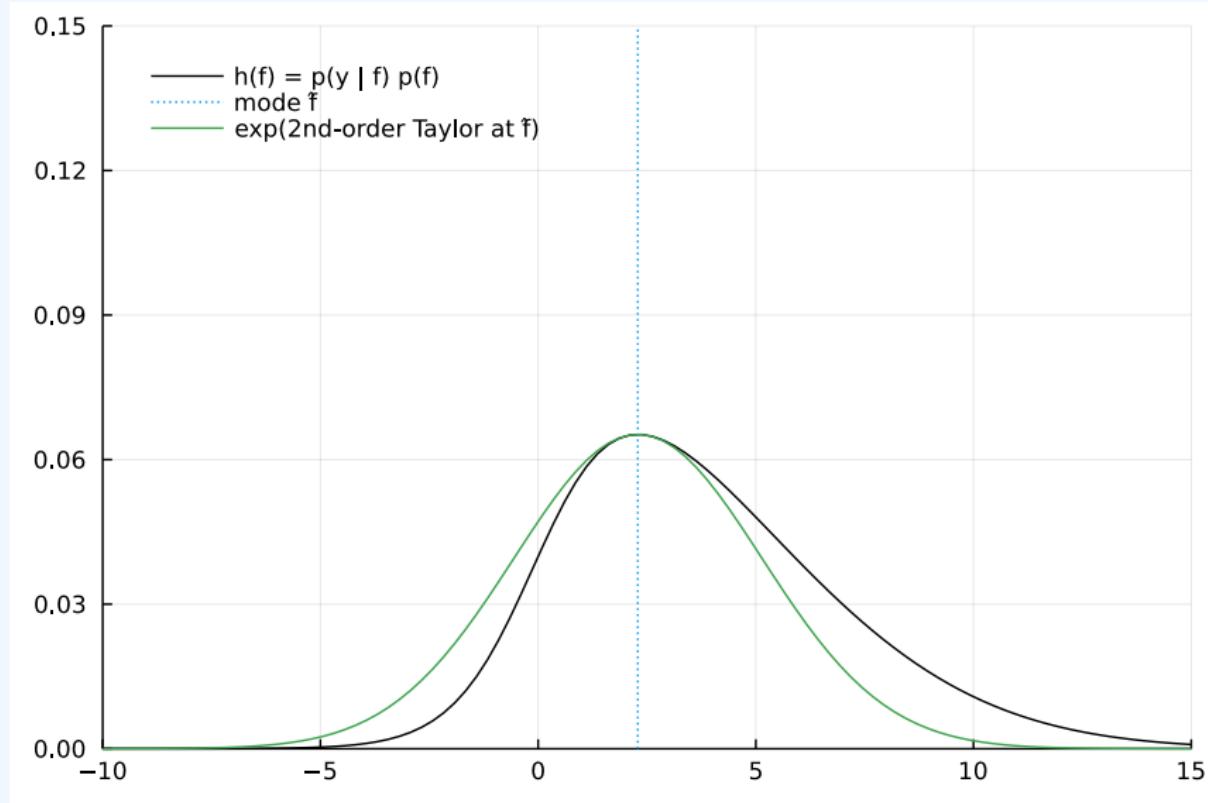
NEWTON'S METHOD



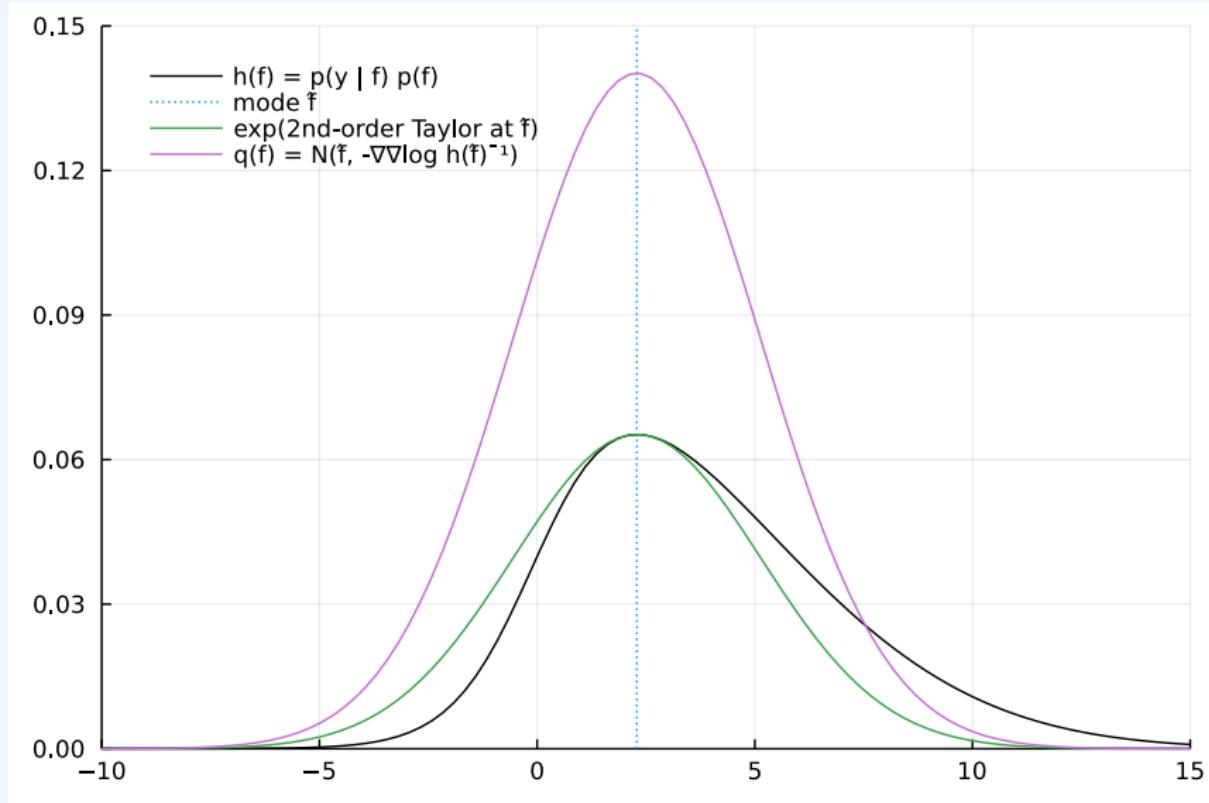
$$\log p(f | y) + \log Z = \log h(f) \approx \mathcal{O}(f^2)$$



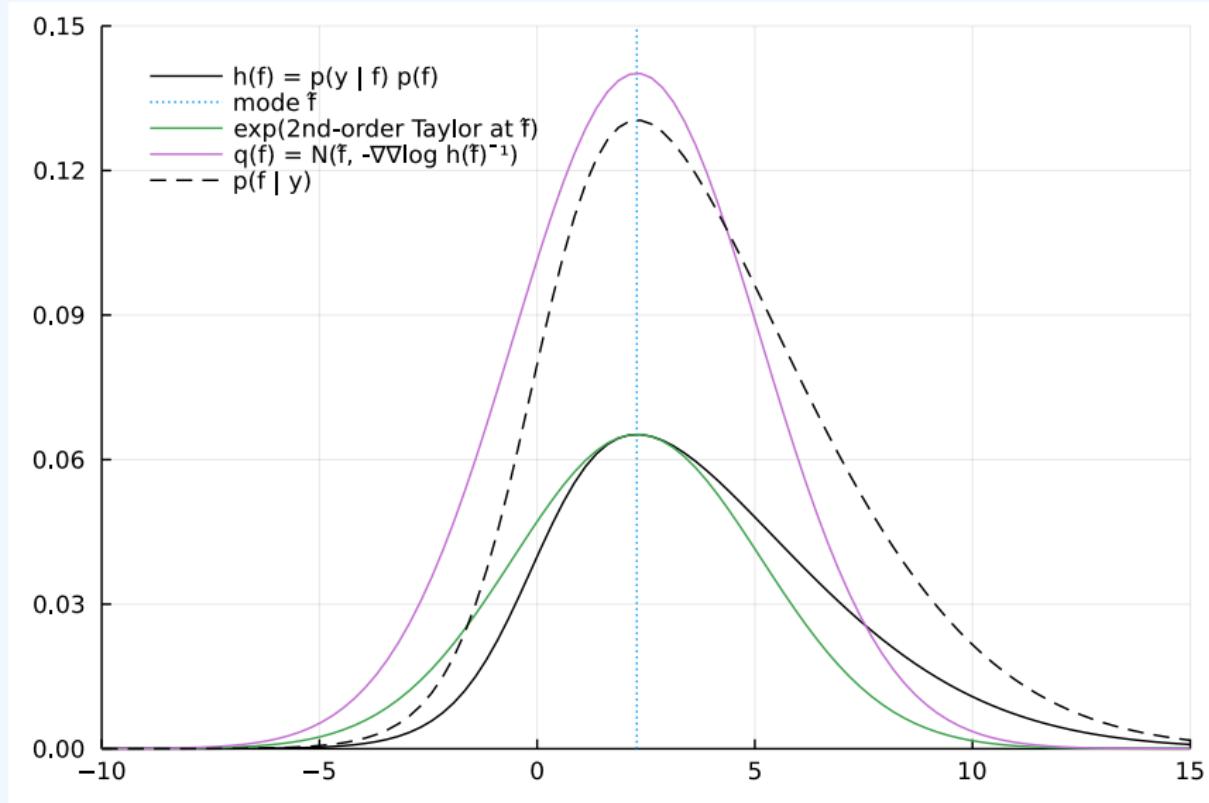
$$p(f \mid y) Z \approx \exp(\mathcal{O}(f^2))$$



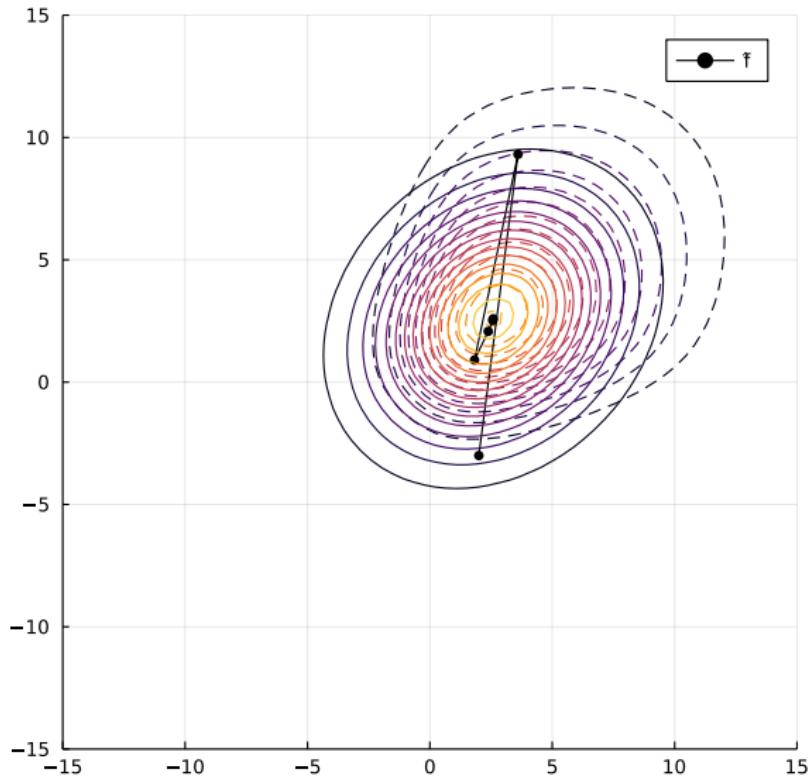
$$p(f | y) \approx \mathcal{N}(f | \hat{f}, -(\mathrm{d}^2 \log h / \mathrm{d}f^2)^{-1})$$



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

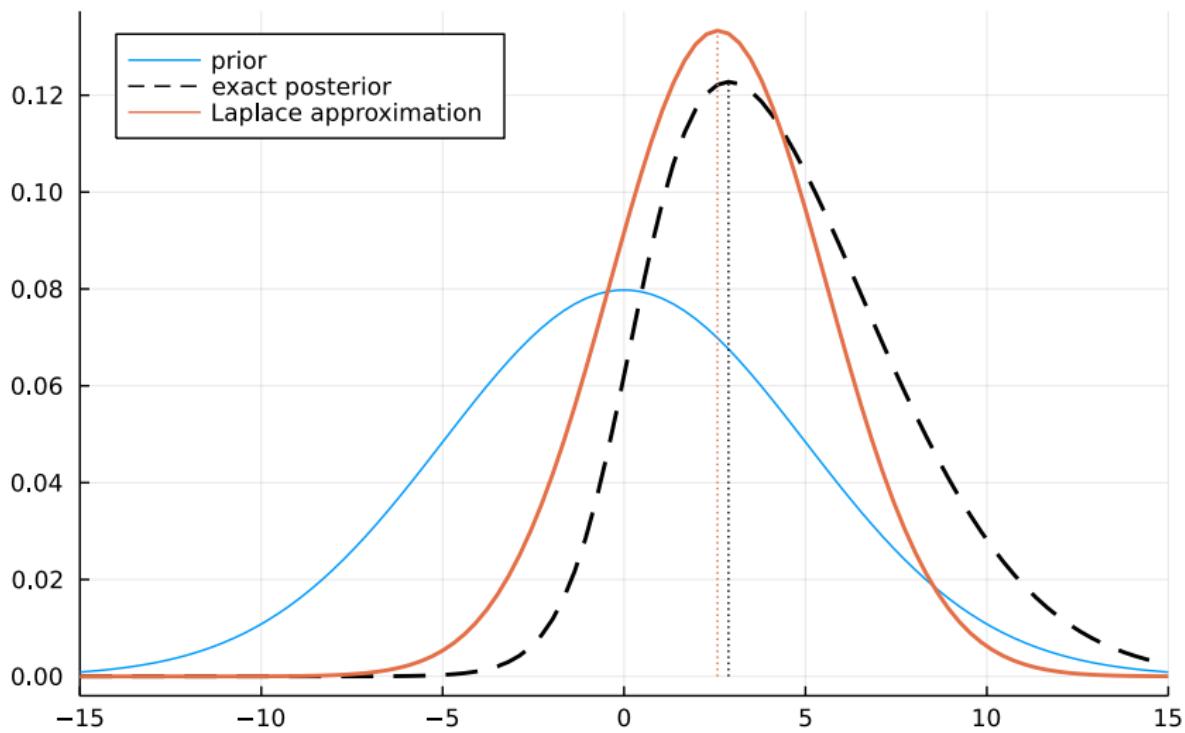


LAPLACE IN 2D EXAMPLE



LAPLACE IN 2D: MARGINALS

marginal of 2D



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 $q(\mathbf{f})$

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

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

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

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

EXPECTATION PROPAGATION (EP)

EXPECTATION PROPAGATION

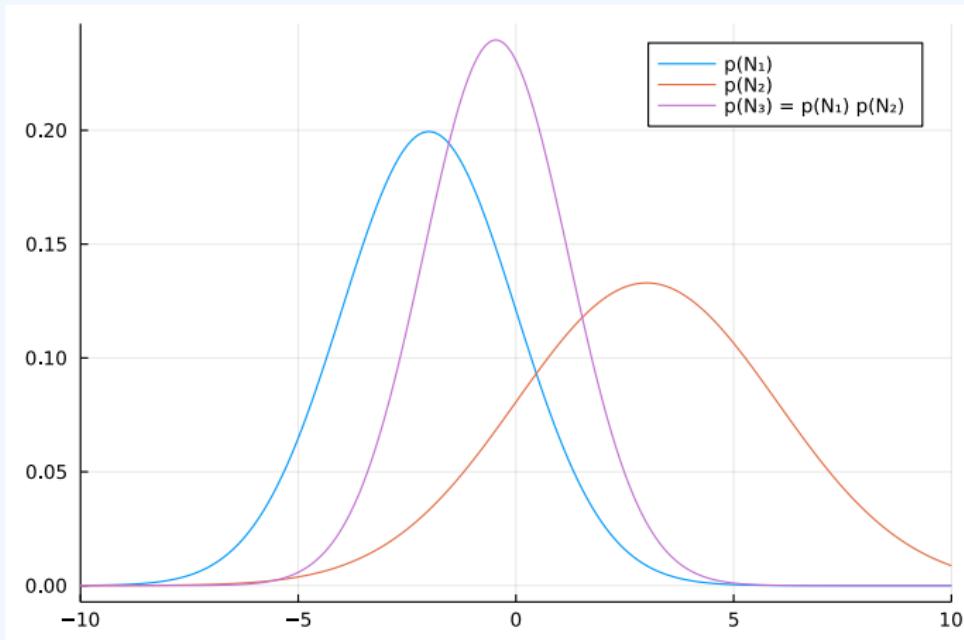
Exact posterior:

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

Approximate posterior:

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

MULTIPLYING AND DIVIDING GAUSSIANS



Adding and subtracting natural (canonical) parameters

EXPECTATION PROPAGATION ITERATIONS

$$\text{"min } \text{KL}[p(\mathbf{f} | \mathbf{y}) \| q(\mathbf{f})]"}$$

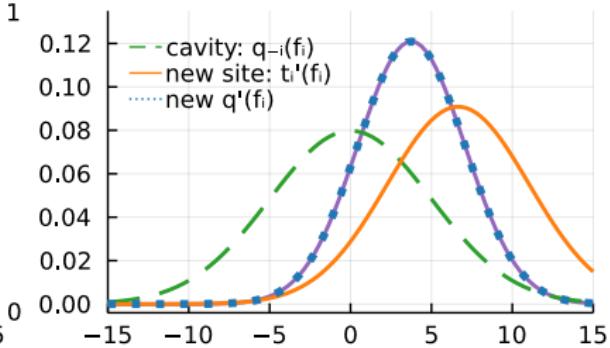
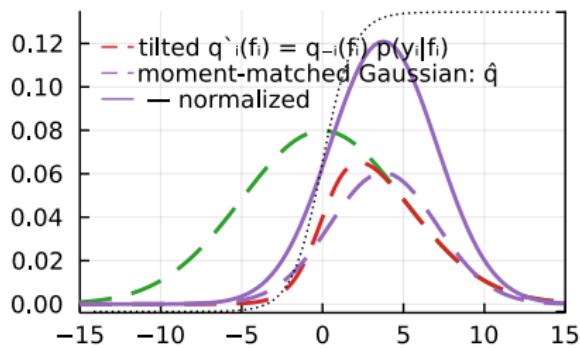
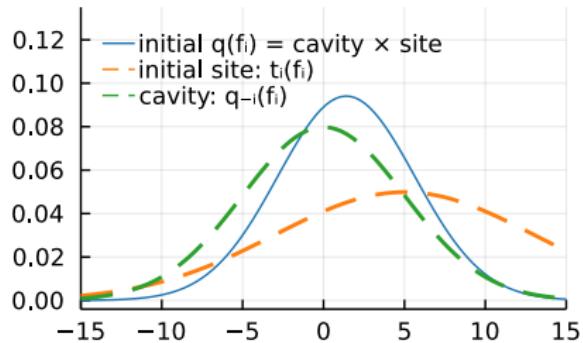
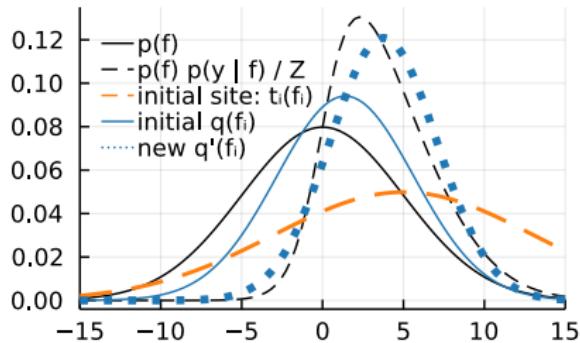
$$q(\mathbf{f}) \propto p(\mathbf{f}) \prod_{i=1}^N \underbrace{t_i(f_i)}_{\text{site } \propto \mathcal{N}(f_i)}$$

For each site i :

1. marginalize $\int q(\mathbf{f}) df_{j \neq i} = q(f_i) \not\propto t_i(f_i)$
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 $\text{argmin} \text{KL}[q_{-i}(f_i) p(y_i | f_i) \| \hat{q}]$ 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)

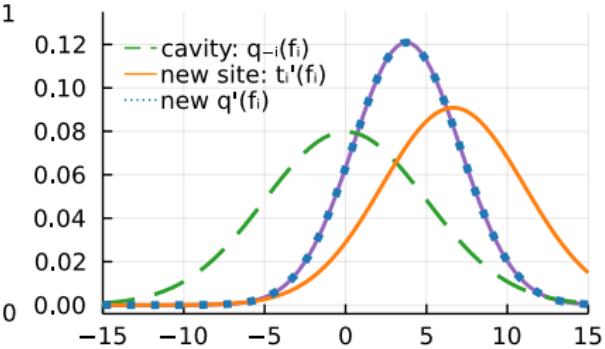
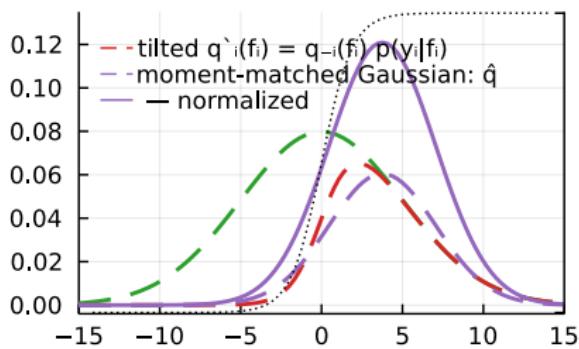
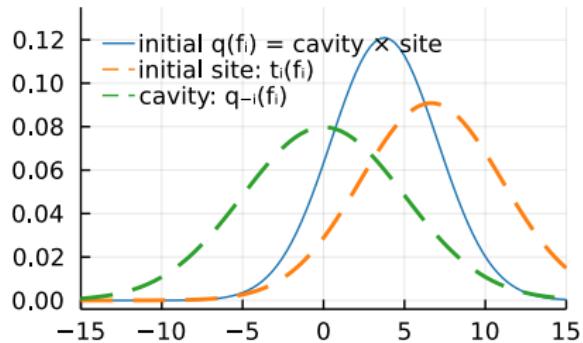
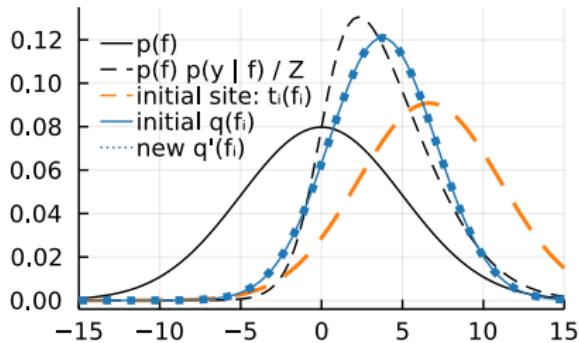
EXPECTATION PROPAGATION IN 1D

iteration 1



EXPECTATION PROPAGATION IN 1D

iteration 2

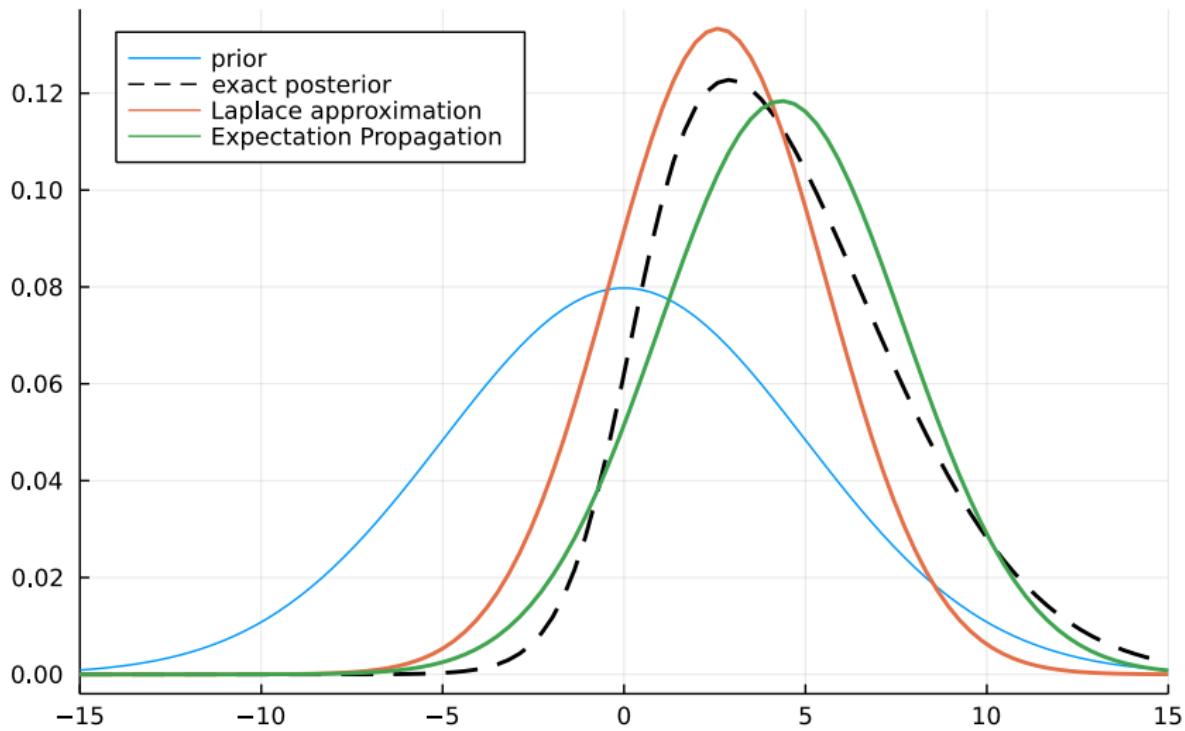


DEMO: EP IN 2D

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

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

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

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

$$= \int q(f) \left[\log \frac{q(f)}{p(f|y)} \right] df = \int q(f) \left[\log q(f) - \log p(f|y) \right] df$$

$$= \int q(f) \left[\log q(f) - \log p(f) - \log p(y|f) + \log p(y) \right] df$$

$$= \int q(f) \left[\log \frac{q(f)}{p(f)} \right] df - \int q(f) \left[\log p(y|f) \right] df + \log p(y)$$

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

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

ELBO

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

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

LIKELIHOOD TERM

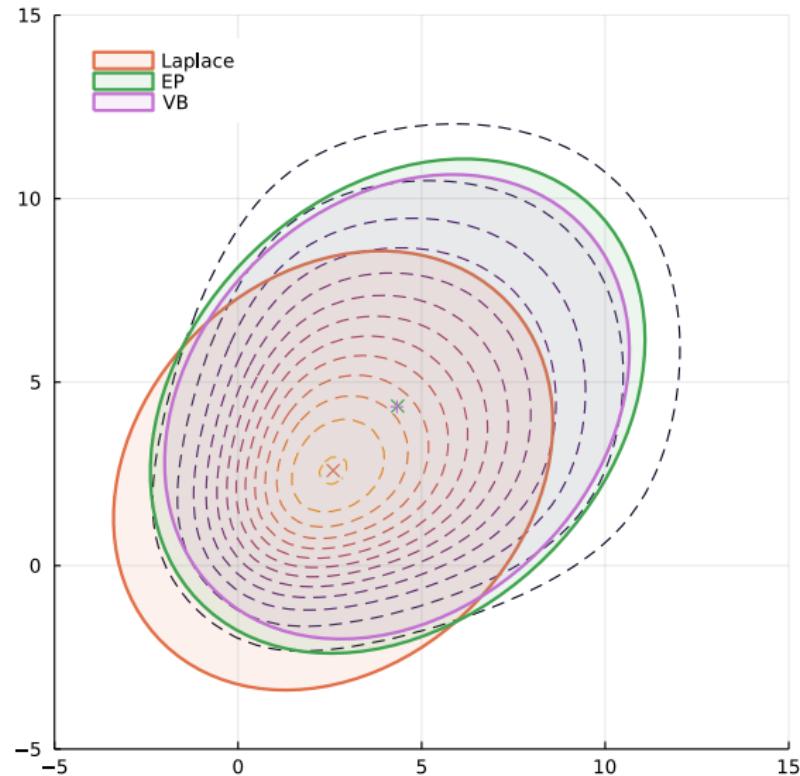
Integral separates for a factorizing likelihood:

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

Evaluating the 1D integrals:

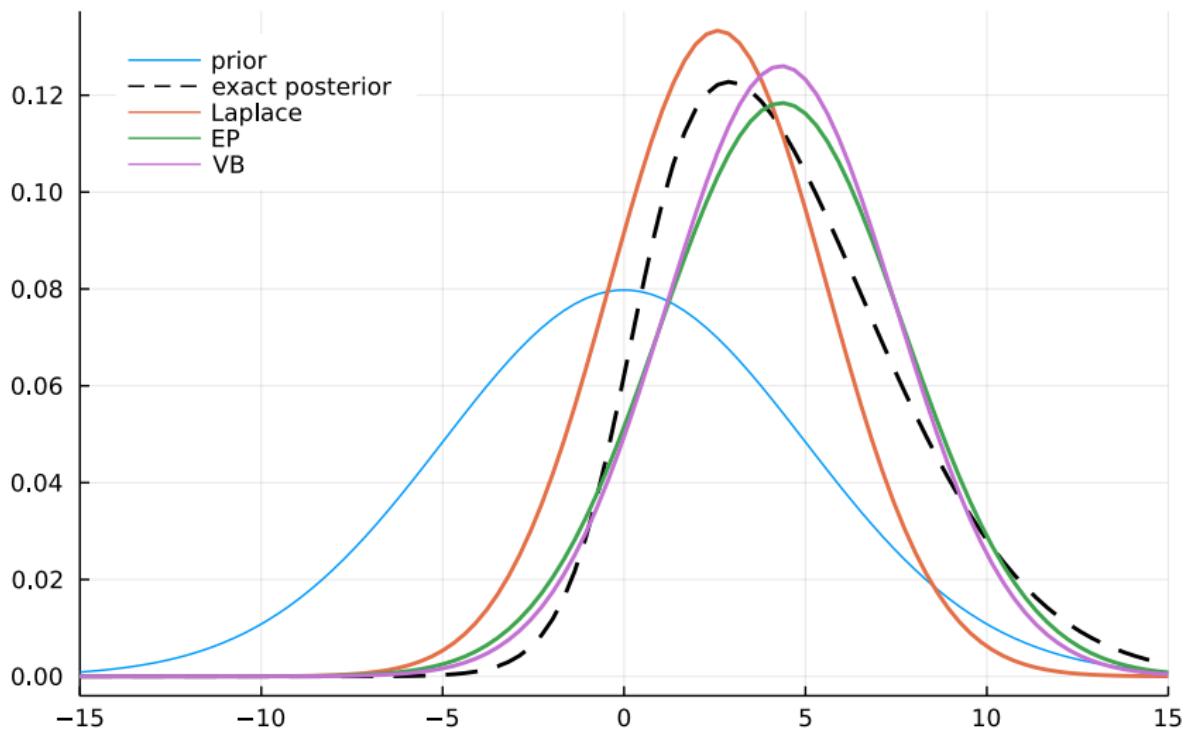
- analytic (e.g. Exponential, Gamma, Poisson)
- Gauss–Hermite quadrature
- Monte Carlo (e.g. multi-class classification)

COMPARISON 2D



MARGINALS

marginal of 2D



VARIATIONAL BAYES: IMPORTANT PROPERTIES

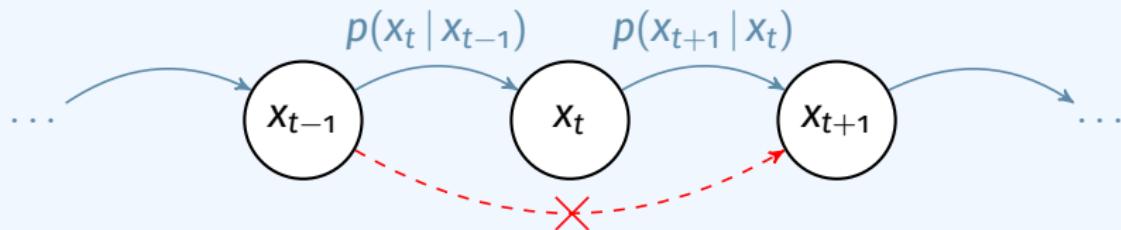
- principled: directly minimising divergence from true posterior
- mode-seeking (e.g. multi-modal posterior: fits just one)
 - + minimises a true lower bound → convergence
 - underestimates variance

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



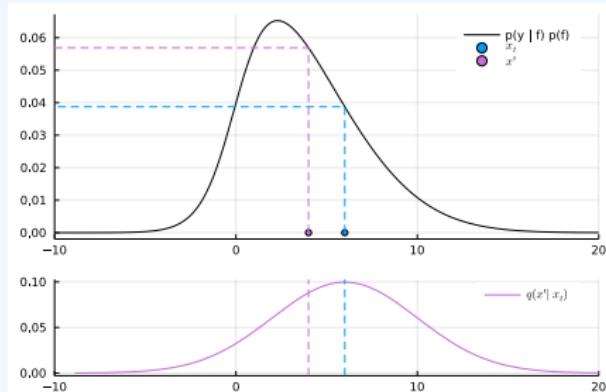
- Samples x_1, \dots, x_T
- “Markov” = 1-step history
- $x_{t+1} \sim p(x_{t+1} | x_t)$, independent of x_{t-1}, \dots, x_1

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 $\frac{h(x')}{h(x_t)}$ → ensures sampling from $p(f | y)$

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

reject: copy $x_{t+1} = x_t$

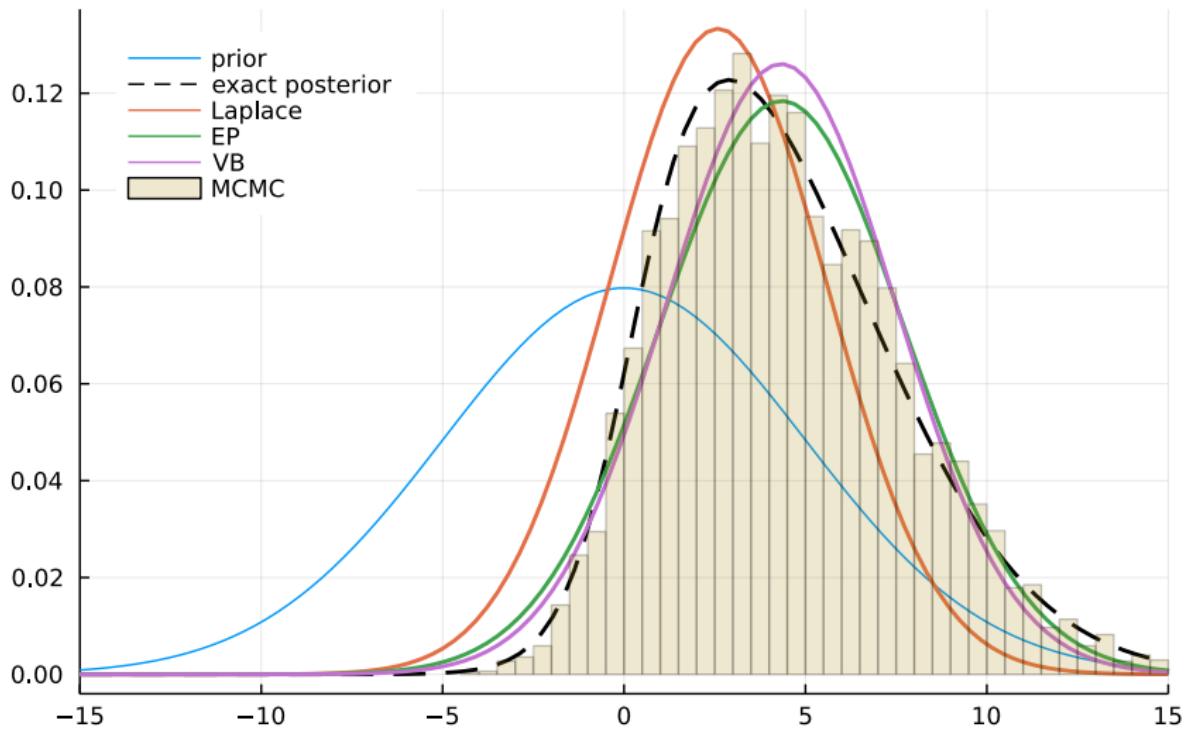
$h(x') > h(x_t)$: always accepts → climbs uphill

DEMO: MCMC IN 2D

tinyurl.com/nongaussian-inference-viz-v1

MARGINALS

marginal of 2D

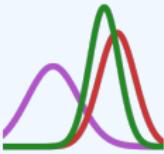


MCMC: IMPORTANT PROPERTIES

- 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 
- TensorFlow Probability (GPflow)  
- Turing.jl 

OUTLINE

- ✓ 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. Comparisons

COMPARISON

COMPARISON

MCMC	Laplace	EP	Variational Bayes
► samples	► \mathcal{N} = curvature at mode	► \mathcal{N} matches marginal moments	► \mathcal{N} minimises $\text{KL}[q(f) \parallel p(f \mid y)]$
► gold standard	► simple & fast	► good calibration in classification	► principled, any likelihood
► slow	► often poor approximation	► may not converge	► underestimates variance

WHAT WE DID NOT COVER...

- Marginal likelihood approximations for hyperparameter learning [6]
- 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]

QUESTIONS!

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