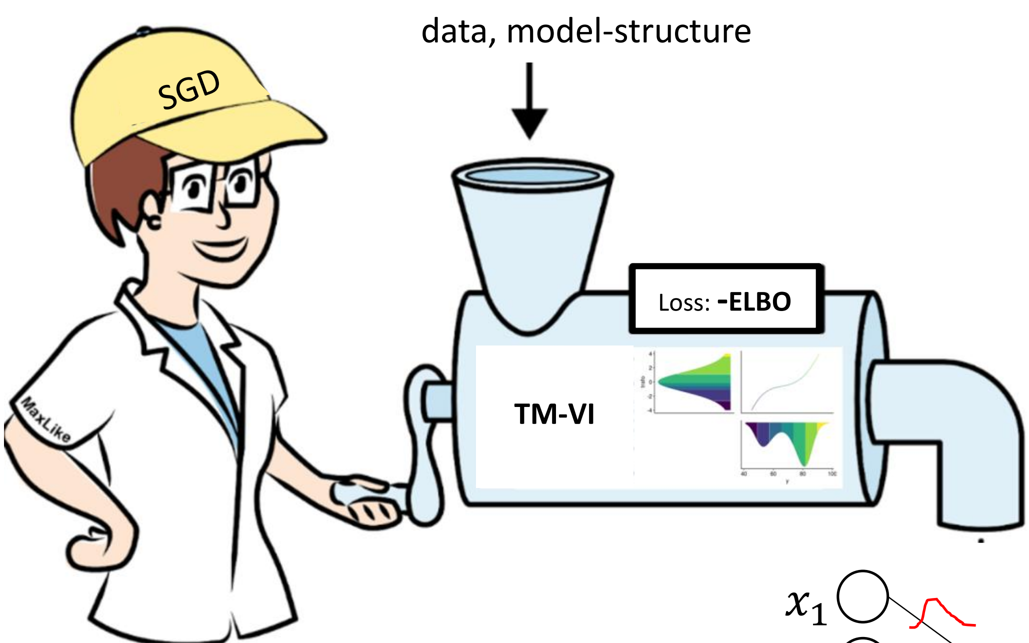
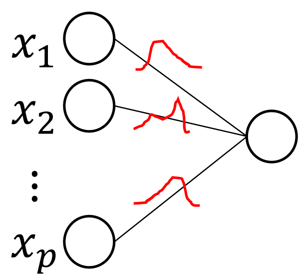
Bayes for dummies

Transformation Models for Flexible Posteriors in Variational Bayes



Goal:
Get a fitted Bayesian model with flexible posteriors for the model parameters



https://arxiv.org/abs/2106.00528

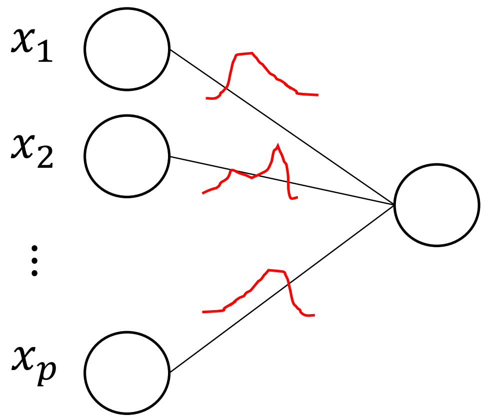
Stefan Hörtling, Daniel Dold, Oliver Dürr, Beate Sick

Prelude

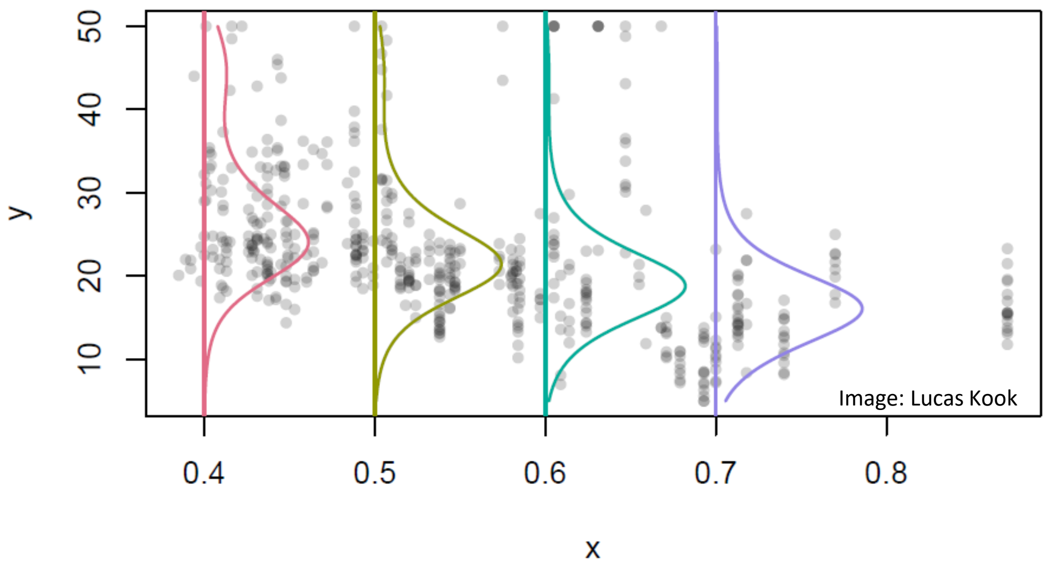
Transformation Models

Modeling complex distributions

complex posteriors



complex conditional probability distributions



Sometimes we need complex distributions and don't know the distribution family.

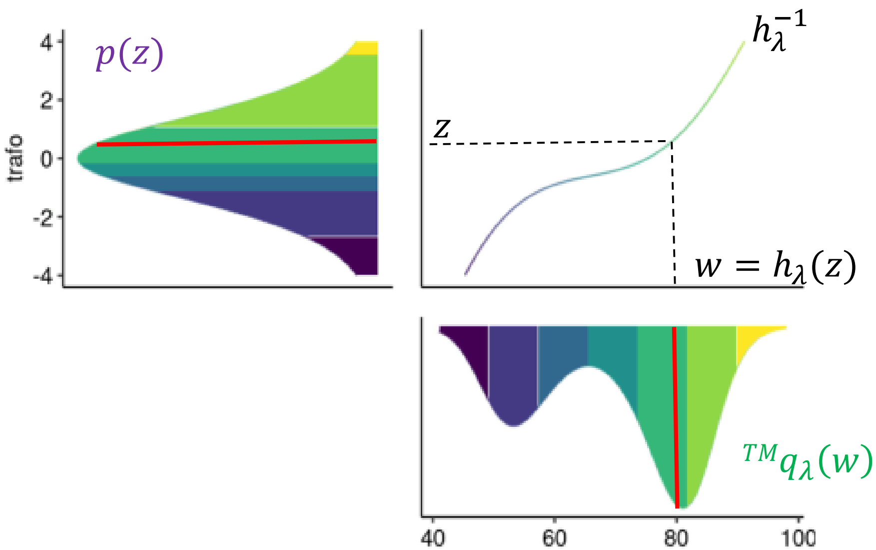
How to model complex distributions?

- Use a mixture model (e.g. mixture Gaussians)
- Use a transformation model!

The idea of transformation models (TM)

The heart of a TM is a **bijective transformation function $\boldsymbol{h_\lambda}$** that transforms between a simple distribution $p(z) = N(0,1)$ and a potentially complex distributional ${}^{TM}q_\lambda(w)$

"change of variable" formula $${}^{TM}q_\lambda(w) = p(z) \cdot \left|\frac{\partial h_\lambda(z)}{\partial z}\right|^{-1}$$



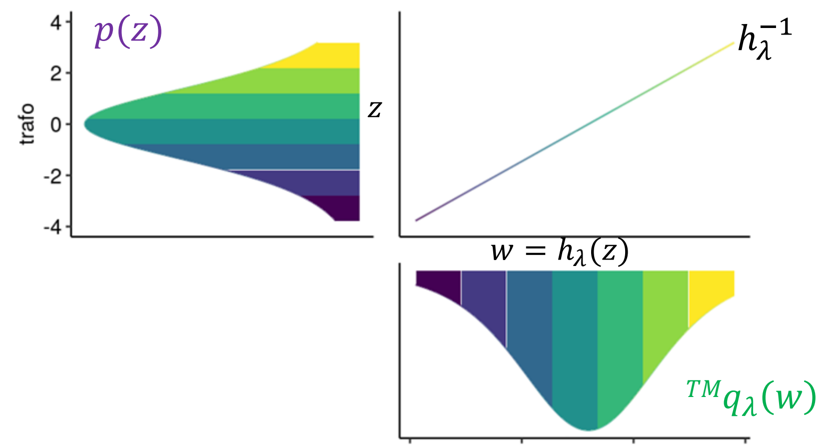


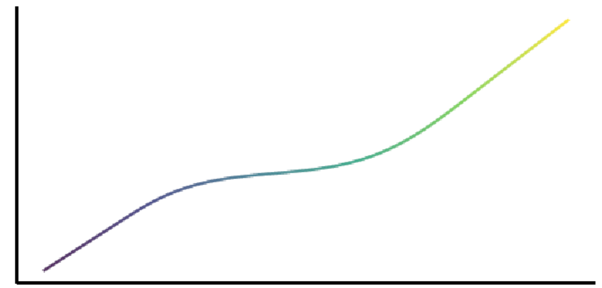
Image: Lucas Kook

Fitting a complex distributions requires a complex transformation function h_λ

Bernstein-polynomial

$$w' = h_\vartheta\,(z') = \sum_{k=1}^{M} \frac{\vartheta_k}{M+1} \mathrm{Be}_k\,(z')$$

$z' \in [0,1]$



A Bernstein polynomial has nice properties:

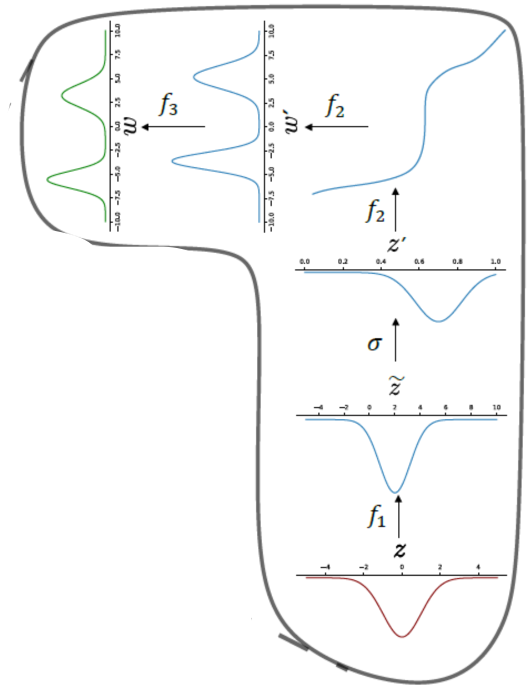
- It can approximate every function on the support $[0;1]$
- It’s flexibility can be controlled by the order M
- It is bijective, i.e. monotone increasing, if parameters $\vartheta_1 \le \vartheta_2 \le \cdots \le \vartheta_M$

Most Likely Transfromation (MLT) 2017 by T.Hothorn, L.Möst, P.Bühlmann https://onlinelibrary.wiley.com/doi/full/10.1111/sjos.12291

Constructing a transformation function

$$f_3(w') = \alpha \cdot w' + \beta$$

$$^{TM}q_\lambda(w) = p(z) \cdot \left|\frac{\partial h_\lambda(z)}{\partial z}\right|^{-1}$$



$$f_2(z') = \sum_{i=0}^{M} \mathrm{Be}_i(z') \frac{\vartheta_i}{M+1}$$

$$f_1(z) = a \cdot z + b$$

$$p(z) = N(0,1)$$

$h_\lambda = f_3 \circ f_2 \circ \sigma \circ f_1$ has M+5 parameters: $\lambda = (a, b, \alpha, \beta, \vartheta_0, \dots, \vartheta_M)$

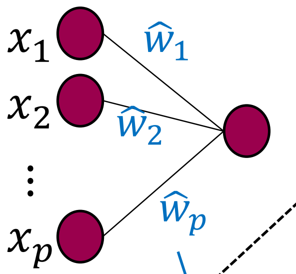
Back to Bayes!

Bayes is often used for probabilistic modeling

Bayesian models allow to capture parameter uncertainty and outcome uncertainty.

<u>Example: Linear regression :</u>

non-probabilistic model

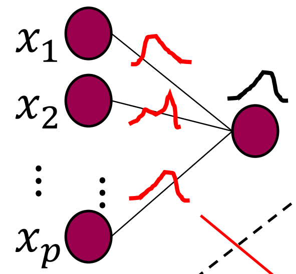


point estimate

$$\hat{\mu}(x) = \sum_{i=1}^{p} \widehat{w_i} \cdot x_i$$

point estimates for
the model parameters

probabilistic Bayesian model



predictive distribution

$$p(\mu|x, D) = \int p(\mu|x, \mathbf{w}) \cdot p(\mathbf{w}|D)\, d\mathbf{w}$$

posterior of the
model parameters

Compute posteriors via Bayes' theorem

posterior

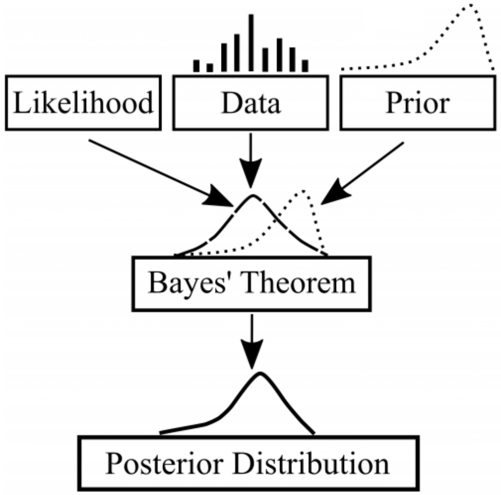
likelihood

pior

$$p(w|D) = \frac{p(D|w) \cdot p(w)}{p(D)} = \frac{p(D|w)p(w)}{\int p(D|w)p(w)dw} \sim p(D|w)p(w)$$

normalizing denominator

this is the most difficult part!



Source: https://towardsdatascience.com/bayesian-statistics-for-data-science-45397ec79c94

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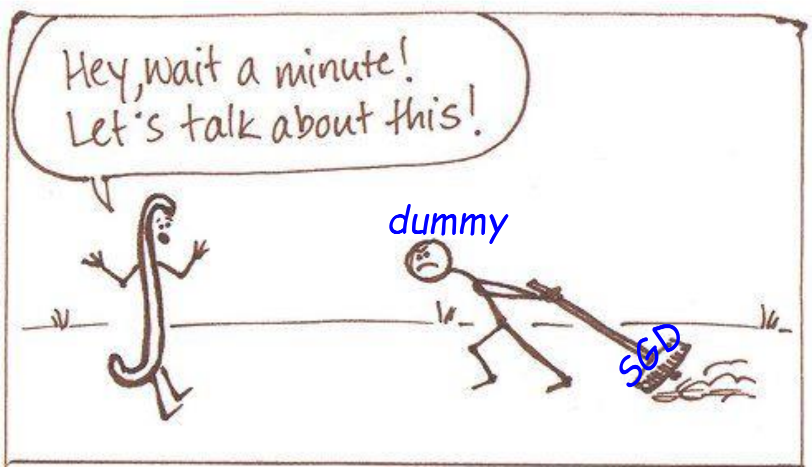


https://brownsharpie.courtneygibbons.org/comic/integrand/

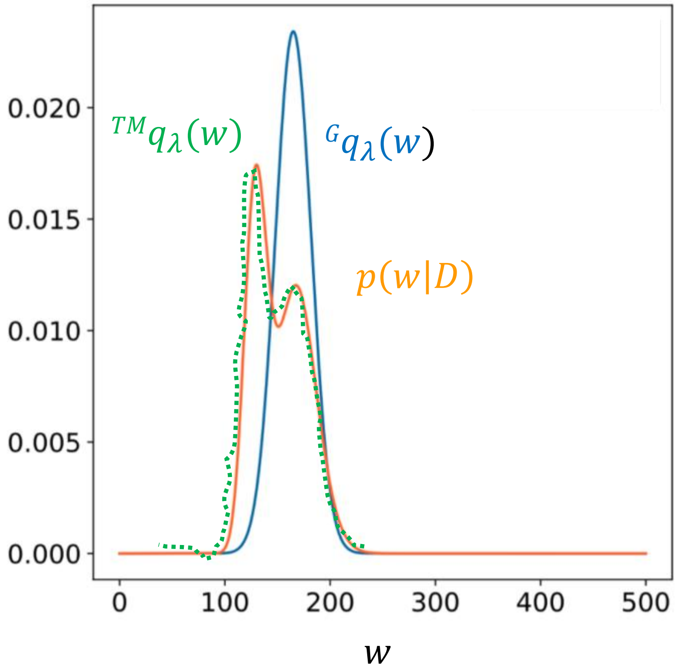
→ Bayes theorem is dead

→ Long live TM-VI

The idea of Variational Inference (VI)

Approximate posterior $p(w|D)$ by a variational distribution $q_\lambda(w)$

- Gaussian-VI: Use a Gaussian as variational distribution ${}^{G}q_\lambda(w)$
- TM-VI: Use a transformation model to get a flexible ${}^{TM}q_\lambda(w)$



Gaussian-VI is not flexible enough to approximate complex posteriors.

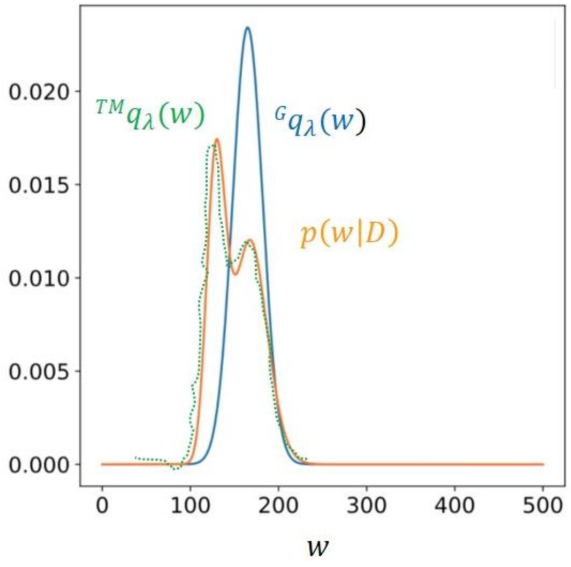
Variational inference is an optimization problem

Find the best q_λ by optimizing parameters $\boldsymbol{\lambda}$ so that

- Kullback-Leibler divergence between variational distribution and posterior distribution is minimized

$$KL(q_\lambda(w)||\mathrm{p(w|D)}) = E_{w\sim q_\lambda}\left(\log\left(\frac{q_\lambda(w)}{\mathrm{p(w|D)}}\right)\right)$$

$$= \log(p(D)) - \underbrace{\left(E_{w\sim q_\lambda}(\log(\mathrm{p(D|w)})) - E_{w\sim q_\lambda}\left(\log\left(\frac{q_\lambda(w)}{\mathrm{p(w)}}\right)\right)\right)}_{\mathrm{ELBO}(\lambda)}$$



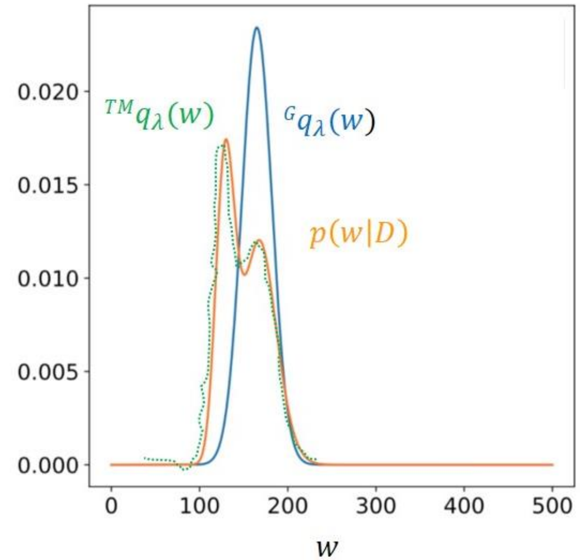
Variational inference is an optimization problem

Task: tune variational parameters $\boldsymbol{\lambda}$ to

- minimize the Kullback-Leibler divergence between variational distribution and posterior distribution

$$KL(q_\lambda(w)||\mathrm{p(w|D)}) = E_{w\sim q_\lambda}\left(\log\left(\frac{q_\lambda(w)}{\mathrm{p(w|D)}}\right)\right)$$

$$= \log(p(D)) - \underbrace{\left(E_{w\sim q_\lambda}(\log(\mathrm{p(D|w)})) - E_{w\sim q_\lambda}\left(\log\left(\frac{q_\lambda(w)}{\mathrm{p(w)}}\right)\right)\right)}_{\mathrm{ELBO}(\lambda)}$$



- $\Leftrightarrow$ maximize the <u>e</u>vidence <u>l</u>ower <u>bo</u>und (ELBO) $\Leftrightarrow$ minimize $\text{loss} = -\mathrm{ELBO}(\lambda)$

0) Initialize λ

1) sample $w_t \sim q_\lambda$

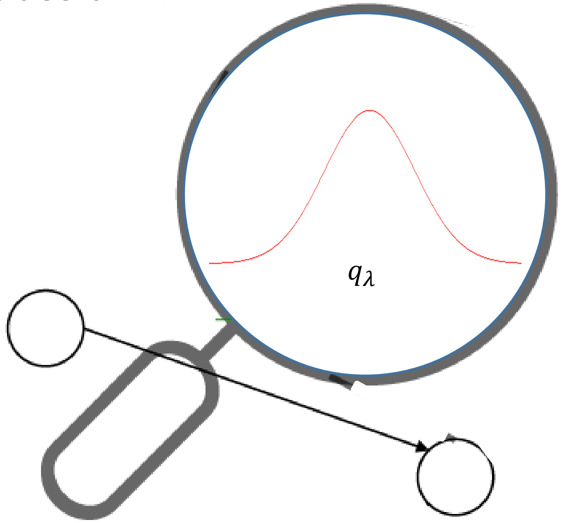
2) $\text{loss} = -\mathrm{ELBO}(\lambda) \approx -\left(\frac{1}{T}\sum_t \log(p(D\,|w_t) - \frac{1}{T}\sum_t \log\left(\frac{q_\lambda(w_t)}{p(w_t)}\right)\right) \overset{SGD}{\Longrightarrow} \lambda_{\text{update}}$

Gaussian-VI versus TM-VI

$${}^{G}q_{\lambda}(w) = N(\mu, \sigma)$$

$${}^{G}\lambda = (\mu, \sigma)$$

Gaussian-VI



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Gauss-VI versus TM-VI

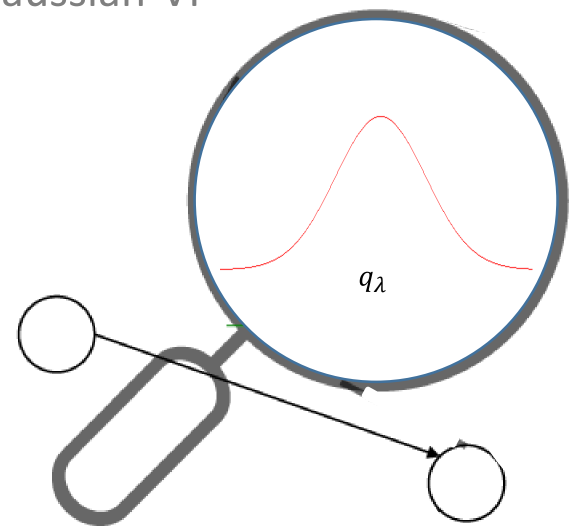
$${}^{G}q_\lambda(w) = N(\mu, \sigma)$$

$${}^{G}\lambda = (\mu, \sigma)$$

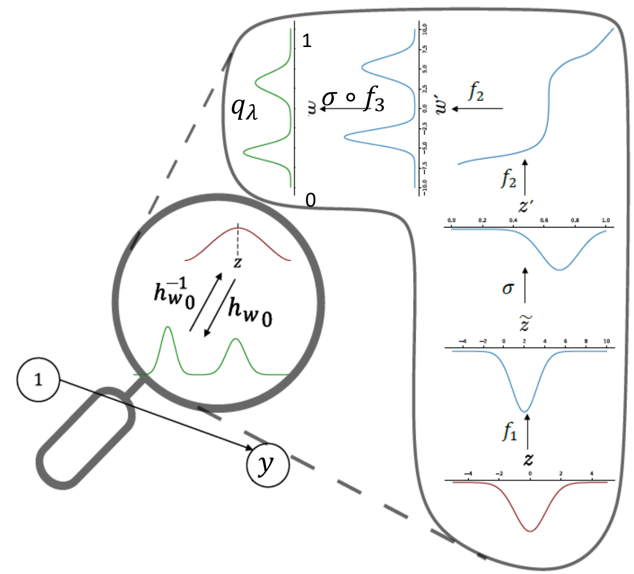
$${}^{G}q_\lambda(w) = p(z) \cdot \left| \frac{\partial h_\lambda(z)}{\partial z} \right|^{-1}$$

$${}^{TM}\lambda = (a, b, \alpha, \beta, \vartheta_0, \dots, \vartheta_M)$$

Gaussian-VI



TM-VI



0) Initialize λ

1) $w_{\text{sample}} \sim q_\lambda$

2) loss $= -\text{ELBO}(\lambda) \overset{SGD}{\Longrightarrow} \lambda_{\text{update}}$

0) Initialize λ

1) $z_{\text{sample}} \sim N(0,1) \Rightarrow w_{\text{sample}} = h_\lambda(z_{\text{sample}})$

2) loss $= -\text{ELBO}(\lambda) \overset{SGD}{\Longrightarrow} \lambda_{\text{update}}$

Single parameter models

Bernoulli experiment as one-parameter-model

Bernoulli model $y \sim \mathrm{Ber}(\pi)$;   two observations $\mathrm{D} = (y_1 = 1, y_2 = 1)$.

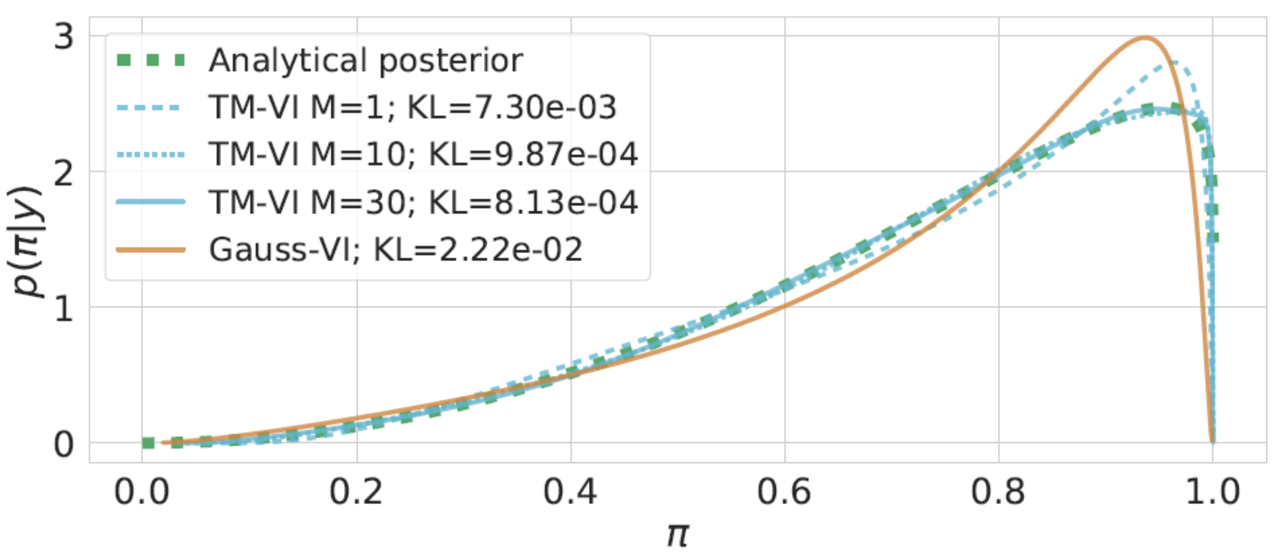
Exact analytical posterior:

Prior: $p(\pi) = \mathrm{Beta}(\alpha = 1.1, \beta = 1.1)$

Likelihood: $\mathrm{p}(D|\pi) = \pi \cdot \pi = \pi^2$

Posterior: $p(\pi|D) = \mathrm{Beta}(\alpha + \sum y_i, \beta + n - \sum y_i)$

$= \mathrm{Beta}(3.3,1.1)$



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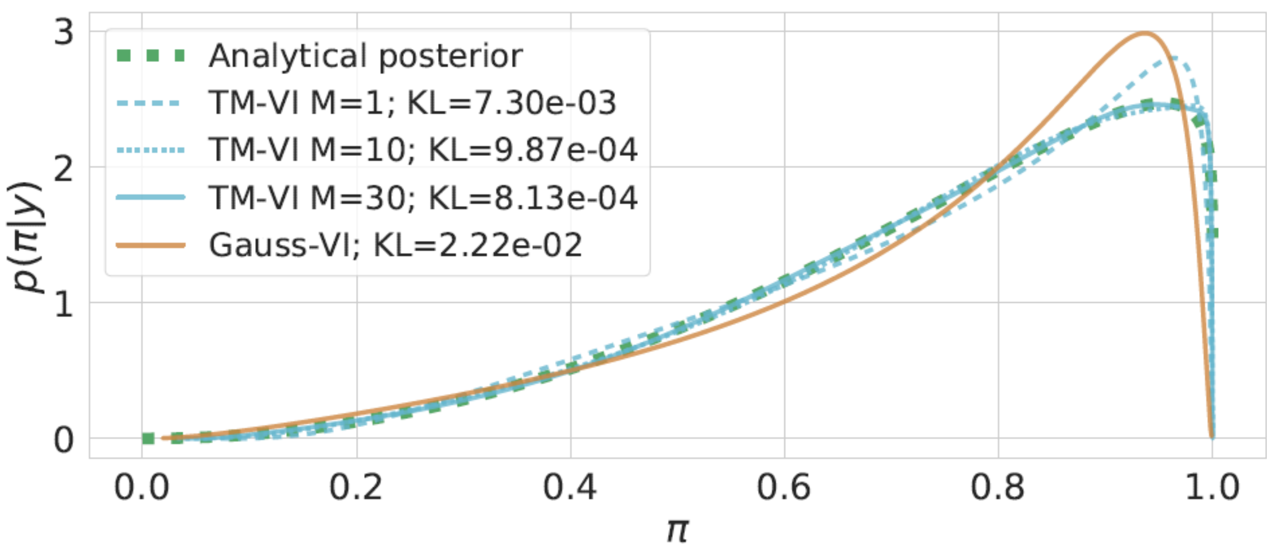
VI-approximated posterior:

Gauss-VI : ${}^{G}q_\lambda(\pi) = \mathrm{sigmoid}(N(\mu, \sigma))$, $\lambda = (\mu, \sigma)$

TM-VI : ${}^{TM}q_\lambda(\pi) = p(z) \cdot \left|\frac{\partial h_\lambda(z)}{\partial z}\right|^{-1}$

$h_\lambda = \sigma \circ f_3 \circ f_2 \circ \sigma \circ f_1, \ \lambda = (a, b, \alpha, \beta, \vartheta_0, \ldots, \vartheta_M)$

loss=$-\mathrm{ELBO}(\lambda) \overset{SGD}{\Longrightarrow} \lambda_{opt} \Rightarrow q_{\lambda_{opt}}$

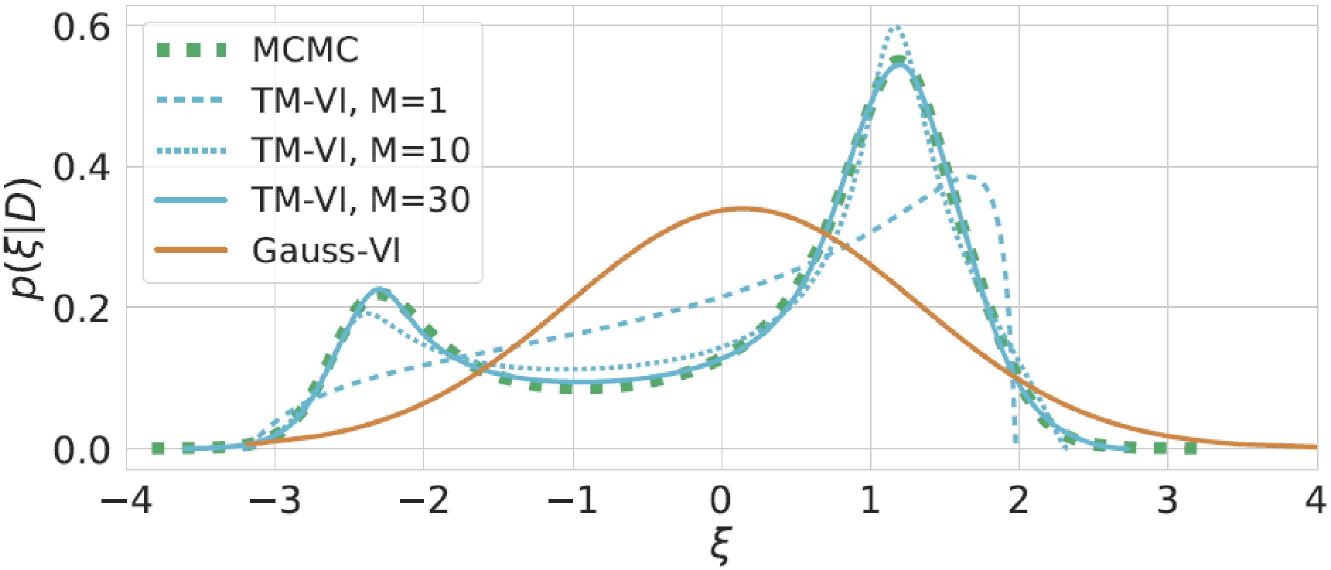


Cauchy experiment as one-parameter-model

Cauchy model $y \sim \text{Cauchy}(\xi; \gamma)$; 6 observations sampled from a mixture-Cauchy

Exact posterior via MCMC (Stan):

```
data{
  int<lower=0> N;
  real<lower=0> gamma;
  vector[N] y;
}
parameters{
  real xi;
}
model{
  y ~ cauchy(xi, gamma);  // likelihood
  xi ~ normal(0, 1);          // prior
}
```



Yao, Y., Vehtari, A., and Gelman, A. The curse and blessing of multimodal posteriors. https://arxiv.org/abs/2006.12335

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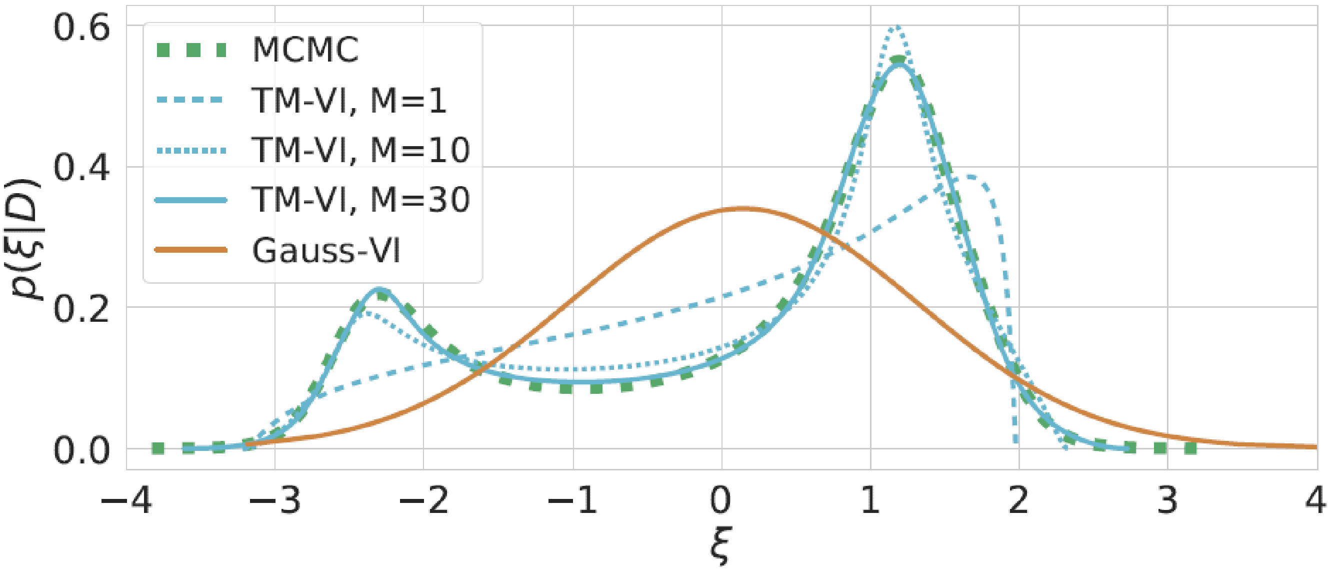

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Multi-parameter models

Mean-field approximation for multi-parameter-models

In **mean-field VI** we assume that we can model all variational distributions independently.

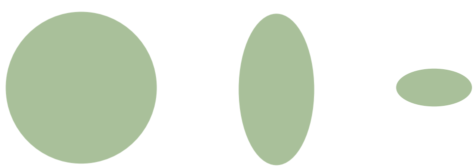
Hence the joint variational distribution is given by a product of marginal distributions:

$$q_\lambda(\boldsymbol{w}) = \prod_{k=1}^{p} q_{\lambda_k}(w_k)$$

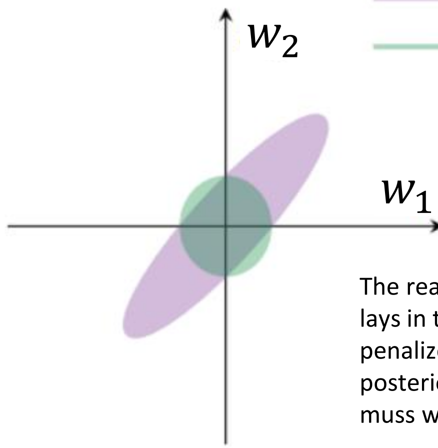
Pros: no need to model dependencies
→ less parameters are needed

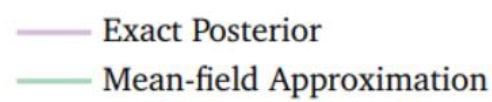
Cons: dependencies are ignored and uncertainty of posterior is underestimated

Possible bivariate Gaussians with mean-field



Impossible bivariate Gaussians with mean-field





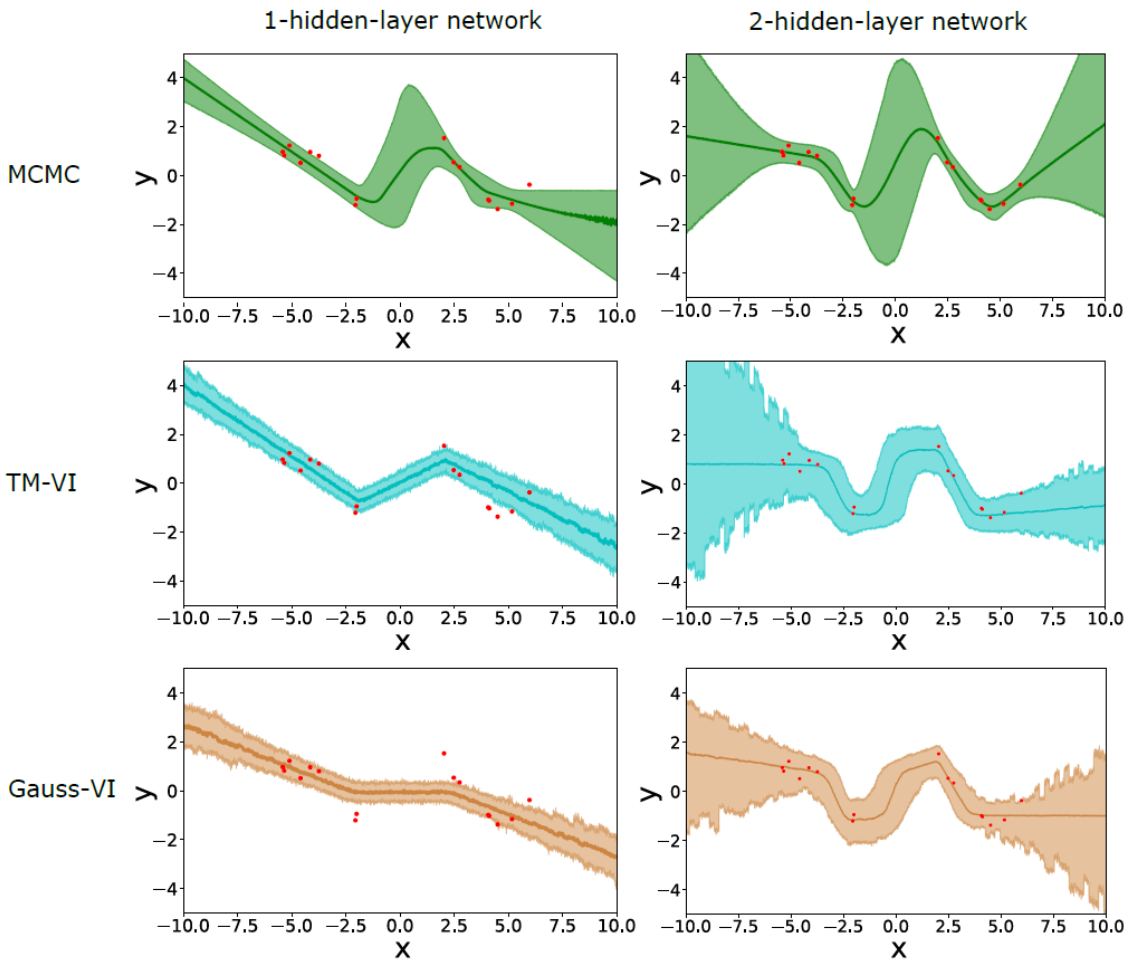
using mean-field Gauss-VI

The reason for the underestimated uncertainty lays in the asymmetry of the KL divergence which penalize more if q_λ puts too much mass where the posterior has little mass, than if q_λ puts too much muss where also the posterior has a big mass.

https://arxiv.org/abs/1601.00670

Mean-field VI for multi-parameter NN

We use Bayesian NNs to estimate the conditional mean $\mu(x)$ of $(y|x) \sim N(\mu(x), \sigma)$



Both VI-approaches underestimate the uncertainty. TM-VI can't leverage in mean-field.

Note: For Gaussian-VI ist known that mean-field does not hurt in deep NN https://arxiv.org/abs/2002.03704

Conclusion and outlook

- VI allows for approximating posterior by an optimization process
- Gaussian-VI approximate posteriors by a Gaussian
- TM-VI allows for flexible posterior approximations
- In single parameter model TM-VI yields very accurate posterior approximations and outperforms Gaussian-VI by far if posteriors are complex
- In multi-parameter models mean-field VI is usually used
- Ignoring dependencies in mean-field VI destroys advantages of TM-VI

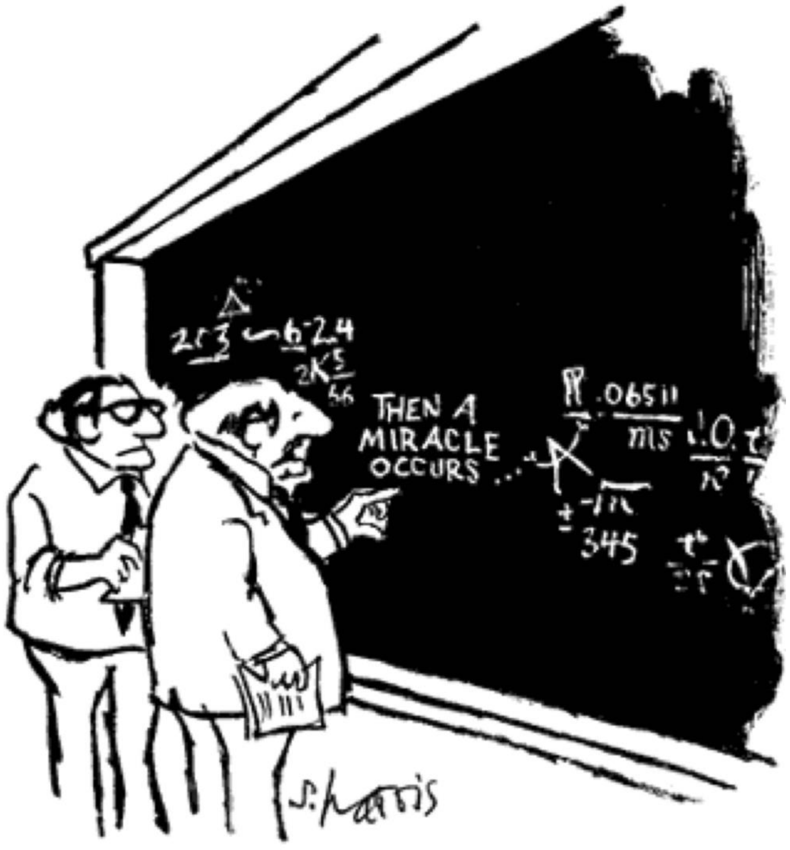
Outlook:

- Go for TM-VI in few-parameter models w/o mean-field approximation
- Go for TM-VI in semi-structured models w and w/o mean-field approximation
- Setup TM-VI-Bayesian transformations models

Appendix

Calculating distance to an unknown function

- We need to calculate KL-Divergence between
  - $p(\theta|D)$ the **unknown posterior**
  - $q_\lambda(\theta)$ and the variational approximation
- Is this possible?



"I think you should be more explicit here in step two."

Be more explicit about step two

$$KL[q_\lambda(\theta)||p(\theta|D)] = \int q_\lambda(\theta)\, log\, \frac{q_\lambda(\theta)}{p(\theta|D)} d\theta$$

We have to start with way, q first

$$p(\theta|D) = p(\theta, D)/p(D)$$

$$KL[q_\lambda(\theta)||p(\theta|D)] = \int q_\lambda(\theta)\, log\, \frac{q_\lambda(\theta)}{p(\theta,D)/p(D)} d\theta$$

$$log(A \cdot B) = log(A) + log(B)$$

$$log(B/A) = -log(A/B)$$

$$KL[q_\lambda(\theta)||p(\theta|D)] = \int q_\lambda(\theta)\, log\, p(D)\, d\theta - \int q_\lambda(\theta)\, log \frac{p(\theta,D)}{q_\lambda(\theta)} d\theta$$

no dependence on θ and $\int q_\lambda(\theta) d\theta = 1$

$$KL[q_\lambda(\theta)||p(\theta|D)] = log\, p(D) - \underbrace{\int q_\lambda(\theta)\, log\, \frac{p(\theta,D)}{q_\lambda(\theta)} d\theta}_{\text{We need to minimize}}$$

Be more explicit about step two (cont'd)

$$\lambda^* = argmin\{- \int q_\lambda(\theta)\, log\, \frac{p(\theta,D)}{q_\lambda(\theta)} d\theta\}$$

$$p(\theta, D) = p(D|\theta) \cdot p(\theta)$$

$$\lambda^* = argmin\{- \int q_\lambda(\theta)\, log\, \frac{p(D|\theta)\cdot p(\theta)}{q_\lambda(\theta)} d\theta\}$$

$$\lambda^* = argmin\{\int q_\lambda(\theta)\, log\, \frac{q_\lambda(\theta)}{p(\theta)} d\theta - \int q_\lambda(\theta) \cdot log\, p(D|\theta)\, d\theta\}$$

$$\lambda^* = argmin\{KL[q_\lambda(\theta)||p(\theta)] - E_{\theta \sim q_\lambda}[log(p(D|\theta)]\}$$

A miracle the unknown posterior $p(\theta|D)$ is gone.