Investigation of Deep Probibalistic Surrogate-models in Bayesian Optimization
in Bayesian Optimization

Master Thesis

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By
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Approval

This thesis has been prepared over six months at the Section for Indoor Climate, Department of Civil Engineering, at the Technical University of Denmark, DTU, in partial fulfilment for the degree Master of Science in Engineering, MSc Eng.

It is assumed that the reader has a basic knowledge in the areas of statistics.

Simon Saugmandsgaard Kruse - s164221

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Signature

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Date

Abstract

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

Acknowledgements

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1 Introduction

Optimization plays an important part in our everyday life, science development, and product design. What different transportation should you choose to get fast from A to B, what songs should land on your playlist, what is the optimal bridge construction. Mathematical optimization problems are all problems on the form,

$$\min_{x \in \mathcal{X}} f(x)$$

where $f : \mathcal{X} \to \mathcal{R}$ is a functional. I.e if it is possible to set up an objective function. e.g. what is the cost of the bridge given a specific design , or how pleasant you think some music, and some constraints such that you keep in the domain of interest. Evaluation of the objective function can be cheap e.g. if it just requires summing and multiplieing numbers or highly expensive if it involves human rating or large simulation and physical experiments. Bayesian optimization is a preferred <ref> framework for the expensive objective functions. And is also referred to as *sample efficient* optimization.

Bayesian optimization is a probabilistic surrogate-based optimization: Assuming some samples from a highly expensive objective a cheap (surrogate) function is used to fit the samples. The next sample is found by minimizing the surrogate and the process is repeated. Bayesian optimization seeks to enhance this procedure with probability theory, where the surrogate function becomes a probabilistic regression model. The most common choice is a Gaussian Process, as it encapsel the uncertainty very well, but also because its inference procedure (computing answers to probability quries like $p(y|x)$) is exact.

Even though GP has proven good for many cases, there will be problems where the assumptions do not hold. In the thesis ... PhD from 2020 he tries out using Bayesian neural networks as surrogate models. This thesis will investigate GP and Bayesian neural networks and try out mixture regression, which might be a even better surrogate model.

<Make a figure of how the parts are all connected>

1.1 notation

Throughout this thesis we will be using Bayesian notation, i.e. $p(x) := P(X = x)$ is the probability density function of the random variable X evaluated in x. and $p(y|x) := P(Y = y|X = x)$ or $p(y|x) := P(Y|X = x)$.

And writing $p(y^2|x)$ means $P(Y^2 = y^2|X = x)$ and **not** $P(Y = y^2|X = x)$

2 Optimization methodology

Given a cost/objective function $f : \mathcal{X} \to \mathbb{R}$, where the domain $\mathcal{X}$ could be a subset of $\mathbb{R}^n$, optimization is a methodology which seeks to find an optimal point, x^*, and value $f^* = f(x)$, given as

$$x^* \in \arg \min_{x \in \mathcal{X}} f(x) \qquad f^* = \min_{x \in \mathcal{X}} f(x) = f(x^*). \tag{2.1}$$

Note that the above formulation is a minimization problem, which is equivalent to a maximization problem maximizing $-f(\cdot)$. Throughout this thesis, we choose to only work with a minimization problem. Solving this problem is intractable except for rare cases e.g. if f is convex and analytically directly solvable or the domain of f is very limited. Hm

> **Example: Direct solution method**
> The unconstrained linear least squares,
>
> $$\min_{x \in \mathbb{R}^n} f(x) := ||Ax - b||_2^2$$
>
> where $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$, is a convex problem, i.e. finding x^* such that $\nabla f(x^*) = 0$ is equivalent to finding the solution to the problem. Assuming $A^T A$ is invertible, linear least squares can be solved directly by the normal equations,
>
> $$\nabla f(x) = 2A^T Ax + 2b^T A = 0 \quad \Leftrightarrow \quad x^* = (A^T A)^{-1} A^T b$$

Most optimization problems are non-convex with multiple local minima. And even if the gradient is given analytically the solution is found among a potentially infinitely large set of stationary points ($\nabla f(x) = 0$) and boundary points - this might be tedious or impossible. When the problem is not directly solvable, mathematical optimization takes an indirect methodology: Design a sequence of experiments that reveal information of the objective function. This information can hopefully lead us to the solution of (2.1). This general way of sequentially solving is presented in the book Bayesian Optimization by Roman Garnett [**bayesoptbook**] and presented here as Algorithm 1.

Algorithm 1 Sequential Optimization [**bayesoptbook**]

    Input: Initial dataset $\mathcal{D}$ ▷ can be empty
    while Temination is not reached **do**
        $x \leftarrow \text{policy}(\mathcal{D})$ ▷ select next observation location
        $y \leftarrow \text{observe}(x)$ ▷ observe objective function at chosen location
        $\mathcal{D} \leftarrow \mathcal{D} \cup \{(x,y)\}$ ▷ update dataset
    return: $\mathcal{D}$

Given data points in the optimization landscape[1] a policy selects a point $x \in \mathcal{X}$ where we make our next observation. Policies can be deterministic or probibalitic, e.g. grid search and random search are examples of policies. The next observation provides us a y value, which combined with x is included to the available data $\mathcal{D}$. Finaly, a stopping criterion decides whether to continue or terminate.

---

[1]"Optimization landscape" defined as the joint set of points in the domain and the objective function evaluated in the points, i.e. $\{(x, f(x)) \in \mathcal{X} \times \mathbb{R} | x \in \mathcal{X}\}$

Example: Grid search

In grid search values along each dimention in $\mathcal{X}$ is seleced and combined with each other, which thereby defines a grid in the parameter space. All points are ordered and systematicly selected. In the content of algorhtim 1 we define the grid search policy as

$$\text{policy}_{GS}(\mathcal{D}) = x_{|\mathcal{D}|+1}$$

assuming $x_1, x_2, \ldots, x_n$ are the ordered grid points and the size of the obtained data is $|\mathcal{D}|$.

Example: Random search

In random search a uniform distribtuion is layed over the domain space $\mathcal{X}$ and a random point is selected from the distribtuion.

$$\text{policy}_{RS}(\mathcal{D}) = x, \quad x \sim p(\mathcal{X})$$

Note that grid search and random search are policies which completely ignores the available data. This is a shame and we can do better.

Example: Gradient descent

Gradient descent is the most simple gradient-based optimization approach. The gradient of a continuous function points in the most ascending direction from the location where it is evaluated. In the minimization task, (2.1), we can iteratively use the opposite gradient direction, i.e. the most descenting directiong. This yields the policy:

$$\text{policy}_{GD}(\mathcal{D}) = x_n - \eta \nabla f(x_n)$$

where we for a brief moment modify y to be a vector, since the observation model is given as:

$$\text{observe}_{GD}(x) = [f(x), \nabla f(x)]$$

Example: Surrogate-based optimization

In surrogate-based optimization all available data is utialised

$$\text{policy}_{sur}(\mathcal{D}) = \min_x \hat{f}(x)$$

2.1 When to use Bayesian optmization

What if $f(x)$ took serval days to evaluate. What if $f(x)$ is noisy? what if discrete points? <more here>

additionally, Bayesian Optimization allow for observation noise,

2.2 Observation model

Many optimization algorhtims assume *exact* evaluations of the objective function. However, this assumption is often wrong especially for objective functions with real-life experiments, imperfect simulations, human interaction where measurement noise is a well known. The observation model is typically noisy and described as

$$y = f(x) + \epsilon$$

Figure 2.1: Hyper parameter tuning of a model $M(\lambda, \sigma)$, 39 evaluation in grid search vs 39 evaluations using Bayesian optimization

where ϵ is the measurement error, this is typically assumed to be Gaussian with zero mean and a variance σ^2 (which could depend on x in a heterostodatic setting) and implies a Gaussian observation model,

$$p(y|x, f(x), \sigma) = \mathcal{N}(y; f(x), \sigma^2)$$

we can extend this model to deal with noiseless observations as well, simply by setting $\sigma = 0$ and let the model colaps into a Direct delta distribution,

$$p(y|x, f(x)) = \delta(y - f(x))$$

i.e. all probability mass for y is on the value $f(x)$ giving the observation sample $y = f(x)$

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3 Bayesian Optimization

Whereas traditional regression workflow is the following: From data, fit model parameters, make predictions using the parameters. The Bayesian framework allows us to skip the dependency of a single set of parameters and instead use all sets of parameters by treating the set of parameters as a random quantity, θ. What is of interest is the predictive posterior distribution,

$$p(y|x, \mathcal{D}) \tag{3.1}$$

Before bringing the parameters/unknown quantities into play, we can ask: What quantities can we play with? This question is answered in two different ways in Gaussian process regression and Bayesian Neural network regression.

3.1 Discriminative model as surrogate model

Discriminative modeling

$$p(y|x)$$

3.2 Using a generative model as surrogate model

Given a generative model over x and y paramitised with θ, we are dealing with the joint distribution

$$p(x, y|\theta)$$

and we are interested in the condtional distribution of y given x,

$$p(y|x, \theta_{y|x})$$

where we have put subscript on θ in order to jump up a level of abstraction since, in fact there is just a mapping between them $\theta_{y|x} := g(\theta, y, x)$

$$p(y|x, \mathcal{D}) = \int p(y|x, \theta_{y|x}) p(\theta_{y|x}|\mathcal{D}) d\theta_{y|x}$$
$$= p(y|x, \hat{\theta}_{y|x})$$

Where the last equation holds as we assume that $p(\theta_{y|x}|\mathcal{D})$ is a delta function i.e. a point estimate with value $\hat{\theta}_{y|x}$. In the case of our Gaussian mixture model, we obtain a point estiamte from the EM algorithm for the variance $\Sigma_{y|k}$, mean value $\mu_{y|k}$ and proportion $\pi_{y|k}$ for each component $k = 1, 2, \ldots, K$

$$\hat{\theta}_{y|x} = (\hat{\Sigma}_{y|k}, \hat{\mu}_{y|k}, \hat{\pi}_{y|k})_{k=1}^{K}$$

However, we are not satisfied with the variance estimate for the regression, as it is way too small for areas with no observed data. It is therefore necessary to manipulate the variance estimate accoring to that observation. We multiply the variance obtained using expectation-maximization on the joint distribution with the inverse of the probability of the data x, and control that the scaling factor is not going wild!

$$\hat{\Sigma}_{y|k} = \Sigma_{y|k}^{GMM} \frac{1}{\max(p(x), 0.01)}$$

In a way this is a manipulation in a Bayesian spirit, as we let prior and subjective knowledge influence the varience prediction.

3.2.1 Inclusion of prior distribution

The conditional distribution $p(y|x)$ is without a prior. Therefore its beliefs is not really ok.. In the flavour of a Poission point process, we introduce the prior..

$$p_{bayes}(y|x) = \frac{p(x) \cdot N \cdot p(y|x) + \lambda p_{prior}(y)}{Z}$$

where the normalization constant Z makes sure the manipulated density integrates to 1, i.e.

$$Z = \int p(x) \cdot N \cdot p(y|x) + \lambda p_{prior}(y) dy = p(x) \cdot N + \lambda$$

<visualization of this!>

mean of $p_{bayes}(y|x)$

$$\begin{aligned} E_{p_{bayes}(y|x)}[y] &= \int y \cdot \frac{f(n, p(x)) \cdot p(y|x) + \lambda p_{prior}(y)}{Z} dy \\ &= \left(p(x) \cdot N \cdot E_{p(y|x)}[y] + \lambda \cdot E_{p_{prior}(y)}[y] \right) \frac{1}{Z} \\ &= \frac{p(x) \cdot N \cdot E_{p(y|x)}[y]}{p(x) \cdot N + \lambda} \end{aligned}$$

variance of $p_{bayes}(y|x)$
We first calculate the second moment,

$$\begin{aligned} E_{p_{bayes}(y|x)}[y^2] &= \int y^2 \cdot \frac{p(x) \cdot N \cdot p(y|x) + \lambda p_{prior}(y)}{Z} dy \\ &= (p(x) \cdot N \cdot E_{p(y|x)}[y^2] + \lambda E_{p_{prior}(y)}[y^2]) \frac{1}{Z} \\ &= \frac{p(x) \cdot N \cdot (Var_{p(y|x)}[y] + E_{p(y|x)}[y]^2) + \lambda Var_{p_{prior}(y)}[y]}{p(x) \cdot N + \lambda} \end{aligned}$$

So the variance is calculated as,

$$V_{p_{bayes}(y|x)}[y] = E_{p_{bayes}(y|x)}[y^2] - E_{p(x,y)}[y]^2$$

implementation
It is not necessary to calculate the conditional distribution, since, using Bayes rule

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

so gives

$$p_{bayes}(y|x) = \frac{p(x) \cdot N \cdot p(y|x) + \lambda p_{prior}(y)}{Z} = \frac{N \cdot p(x,y) + \lambda p_{prior}(y)}{Z}$$

$$E_{p(x,y)}[y] = \int_y \int_x y p(x,y) dx dy = \int_y y p(y) dy = E_{p(y)}[y]$$

3.3 Acquisition function

A popular choice of acquisition function is expected improvement:

$$\mathbb{E}_{y_*|\mathbf{x}_*, D_n}[\min(0, y_{\min} - y_*)] = ??$$

$$\mathbb{E}[\min(0, y_{\min} - y_*)|\mathbf{x}_*, D_n] = \int_{-\infty}^{\infty} \min(0, y_{\min} - y_*) p(y_*|\mathbf{x}_*, D_n) dy_*$$

$$= \int_{-\infty}^{y_{\min}} (y_{\min} - y_*) p(y_*|\mathbf{x}_*, D_n) dy_*$$

$$\approx \frac{1}{N} \sum_{\theta \in \Omega} [y_{\min} - f_\theta(x)],$$

where $\Omega = \{\theta | f_\theta(x) < y_{\min}\}$

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4 Bayesian regression models - probabilistic surrogate model

As mentioned in the previous sections, the first of two repeated steps in Bayesian optimization is to create a good Bayesian regression model. i.e. finding the probility of prediction for a arbitrary point x given datapoints $\mathcal{D} = \{x_1, y_1, \ldots, x_n, y_n\}$,

$$p(y|x, \mathcal{D})$$

The surrogate model of choise in Bayesian optimization is a Gaussian Process, and Bayesian Neural Network. These are discriminative models, however, another approach, which we focus on in this project, is to model y and x jointly in a so-called generative model.

4.1 Gaussian mixture regression

Taking a convex combination of a set of multivariate Gaussian distributions is a Gaussian mixture model

$$p(z) = \sum_{k=1}^{K} \pi_k \mathcal{N}(z|\mu_k, \Sigma_k)$$

Defining $z := (x, y)$ we can model our data, as a generative model $p(x, y)$, now, since the conditonal of a Gaussain mixture again is Gaussain mixture - i.e. closed form expression, we can exactly calculate $p(y|x) = GMM_{y|x}$

Assuming iid data the likelihood is given as

$$p(\mathcal{D}|\mu_1, \ldots, \mu_K, \Sigma_1, \ldots, \Sigma_K, \pi_1, \ldots, \pi_K) = \prod_{i=1}^{n} \sum_{k=1}^{K} \pi_k \mathcal{N}(z_i|\mu_k, \Sigma_k)$$

And the log likelihood,

$$\log p(\mathcal{D}|..) = \sum_{i=1}^{n} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(z_i|\mu_k, \Sigma_k)$$

4.2 Mixture regression in a Bayesian setting

As seen in examples. The uncertainty of conditional distribution is way too certain in areas with no data points, therefore we need to enhance the model with some bayesian flavour.

$$p(y|x, \mathcal{D}) = p(y|x, Z)p(Z|x)$$

Expetation-maximization algorithm
A way to find local maxima in the likehood function is using the EM algorithm.

If we define a latent/hiddem random variabel $Z_i \in \{1, \ldots, K\}$ for each data point, then the likelihood function becomes,

$$L(\theta|\mathcal{D}, Z) = \prod_{i=1}^{n} \sum_{k=1}^{K} 1(Z_i = k)\pi_k \mathcal{N}(z_i|\mu_k, \Sigma_k)$$

Now the expectation wrt. the current value $p(Z|\mathcal{D}, \theta^k)$ is given as

$$Q(\theta|\theta^k) = \mathcal{E}_{p(Z|\mathcal{D},\theta^k)} = L(\theta|\mathcal{D}, Z)$$

And then update the next parameter estimate with

$$\theta^{k+1} = \arg\max_{\theta} Q(\theta|\theta^k)$$

This is repeated untill convergence.

4.3 Sum product networks

We will for a large extend just see SPN as a large mixture model. This is a totally valid observation.

Mixture model

Definition 1 *A sub-network $\bar{S}_z$ of S is an SPN, which includes the root S and then includes nodes according to the following recursive scheme:*

Collection of sub-network S_z of S

---

    function Process(node i, S_z)
        if $i \in \mathcal{L}eaf(S)$ **then**
            return:
        if $i \in \mathcal{S}um(S)$ **then**
            $S_z = S_z.add(j \in ch(i))$ ▷ include one child of node i
            return: Process(j, S_z)
        if $i \in \mathcal{P}rod(S)$ **then**
            $S_z = S_z \cup \{j | j \in ch(i)\}$ ▷ include all childen of node i
            for $j \in ch(i)$ **do**
                return: Process(j, S_z)
        return: S_z
    $S_z = $ Process(root,∅)

So we see that at each sum node the number of different sub-networks multiplies with the number of children for that sum node. And thereby, the total number of sub-networks is

$$Z = \prod_{i \in \mathcal{S}um(S)} |ch(i)|$$

i.e. an exponential large amount of sub-networks. This is the amount of mixture components implicitly defined in an SPN. Denote the set of edges in the sub-network $\mathcal{E}(S_z)$. Now the we define a mixture coeficient, λ_z and component for each S_z as

$$\lambda_z := \prod_{(i,j) \in \mathcal{E}(S_z)} w_{i,j}, \qquad p_z(x, y|\theta) := \prod_{i \in \mathcal{L}(S_z)} p_i(x, y)$$

where $p_i(x, y)$ is the leaf distribution at leaf node i paramitised with θ. It can now be proven that the SPN can be interpreted as the following mixture model,

$$p(x, y|w, \theta) = \sum_{z=1}^{Z} \lambda_z(w) p_z(x, y|\theta)$$

i.e. by the weighted sum of all Z sub-networks. For convinience we define each sum component as $p(z, x, y|w, \theta) := \lambda_z(w) p_z(x, y|\theta)$. Evaluation of $p(x, y|w, \theta)$ will never be done as the sum over Z components, instead there is a proposition.

Proposition 1 *Consider a SPN, S, a sum node $q \in \mathcal{S}um(S)$ and a child $i \in ch(q)$, then the following relation holds,*

$$\sum_{z:(q,i)\in\mathcal{E}(S_z)} \lambda_z(w)p_z(x,y|\theta) = w_{i,q}\frac{\partial S}{\partial v(q)}v(i)$$

Conditional of SPN

We will soon see how it is possible to write the conditional distribution as the mixture,

$$p(y|x) = \sum_{z\in\Sigma(S)} \gamma(x)p_{z_y}(y)$$

where $\Sigma(S)$ is the set of all sub-networks in the SPN, S - IT IS EXPONENTIALLY LARGE. And where $p_{z_y}(y)$ is defined through $p_z(x,y)$,

$$p_z(x,y) = \prod_{l\in\mathcal{L}eaf(z_x)} \phi_l(x) \prod_{l\in\mathcal{L}eaf(z_y)} \phi_l(y)$$
$$=: p_{z_x}(x)p_{z_y}(y)$$

where ϕ_l is the density of the l'th leafs tractable distribution. Recall that we can interpret an SPN as the mixture model,

$$p(x,y) = \sum_{z\in\Sigma(S)} \lambda_z p_z(x,y)$$

where $\lambda_z = \prod_{(q,j)\in\mathcal{E}(z)} w_{q,j}$. First we calculate the marginal density, $p(x)$,

$$p(x) = \int p(x,y)dy$$
$$= \int \sum_{z\in\Sigma(S)} \lambda_z p_z(x,y)dy$$
$$= \sum_{z\in\Sigma(S)} \lambda_z p_{z_x}(x) \int p_{z_y}(y)dy$$
$$= \sum_{z\in\Sigma(S)} \lambda_z p_{z_x}(x)$$

Now we are ready to calculate the conditional density,

$$p(y|x) = \frac{p(x,y)}{p(x)}$$
$$= \frac{\sum_{z\in\Sigma(S)} \lambda_z p_z(x,y)}{p(x)}$$
$$= \sum_{z\in\Sigma(S)} \frac{\lambda_z p_{z_x}(x)}{p(x)}p_{z_y}(y)$$
$$= \sum_{z\in\Sigma(S)} \frac{\lambda_z p_{z_x}(x)}{\sum_{z\in\Sigma(S)} \lambda_z p_{z_x}(x)}p_{z_y}(y)$$
$$= \sum_{z\in\Sigma(S)} \gamma(x)p_{z_y}(y)$$

So we defined $\gamma(x) = \frac{\lambda_z p_{z_x}(x)}{\sum_{z\in\Sigma(S)} \lambda_z p_{z_x}(x)}$ and this is very convinient, as we will see soon is equavalent to the derivative of the log-likelihood of the SPN, which is easily obtained by automatic differentiation.

calculation of $\gamma(x)$

expectation maximization of a mixture model, is given by Bishop.. the responsibility of a datapoint to belong to one mixture component, is given by

$$\gamma(z_{nk}) = \frac{w_k p_j(x_n)}{\sum_i w_i p_i(x_n)}$$

We can prove that the responsibility is equal to the gradient of the log likelihood,

$$L := \sum_n \log \sum_j w_j \exp \psi_j(x_n)$$

where we define $\psi_j(x_n) = \log p_j(x_n)$. Take the gradient

$$\frac{\partial L}{\partial \psi_j(x_n)} = \frac{w_k p_j(x_n)}{\sum_i w_i p_i(x_n)}$$

Note that the gradient easily can be found using autograd.

Mean and variance of $p(y|x)$

The mean of the conditional is just

$$E_{p(y|x)}[y] = \sum_{z \in \Sigma(S)} \gamma(x) \int y p_{z_y}(y) dy$$
$$= \sum_{z \in \Sigma(S)} \gamma(x) \prod_{l \in \mathcal{L}eaf(z_y)} E_{\phi_l}[y]$$

and the variance is found using the second moment,

$$E_{p(y|x)}[y^2] = \sum_{z \in \Sigma(S)} \gamma(x) \int y^2 p_{z_y}(y) dy$$
$$= \sum_{z \in \Sigma(S)} \gamma(x) \prod_{l \in \mathcal{L}eaf(z_y)} (Var_{\phi_l}[y] + E_{\phi_l}[y]^2)$$

SPN is an exponential large mixture model, with linear inference - unlike GMM. !? Write naive bayesian mixture model as a Sum Product Network

sum nodes play a role of mixtures over their children distribution, similar to a classic mixture model

Product nodes on the other hand, are equivalent to factorizations over independent distributions as they are combining disjoint RVs.

SPNs can also be interpreted as deep feed forward neural network [@vergari]. Here, imagine the weights of the sum nodes are parameters, leaf distributions are input neurons, root node is output and all other nodes correspond to hidden neurons

5 Inference: Prediction and learning

Inference is the process of computing answers to queries about a probabilistic model after observing data. In Bayesian regression, the query is the predictive distribution, $p(y|x, \mathcal{D})$, as we are interested in the distribution of y given x and already observed data, $\mathcal{D}$. This often indirectly create the posterior query, $p(\theta|\mathcal{D})$, the probability of model parameters θ given data $\mathcal{D}$. Lastly it is also inference, when we train a Gaussian mixture model or SPN using the expectation-maximization algorithm (EM), since we are iteratively answering the query $E_{p(z|\theta^{(k)})}[z|\theta]$.

5.1 Exact and approximate inference

We distinguish between two different ways of inference, exact and approximate inference. It is *exact inference* when a probabilistic query is calculated exact. It is possible to calculate exact inference on the predictive distribution for the Gaussian mixture model, Sum product network, and Gaussian processes. Models which allow for exact inference have a powerful advantage over the models with approximate inference since we can guarantee the answers to the queries are correct, however, they are usually also less expressive. It is possible to make exact inference of SPN, Gaussian Process, and Gaussian Mixture Regression.

When it is not possible to answer a probabilistic query exact, we can approximate the answer using *approximate inference*. When dealing with complicated and expressive statistical models, exact inference is often intractable and we need to use approximate inference. Approximate inference is a broad category of methods, which includes variational inference, Laplace approximation, and Markov chain Monte Carlo (MCMC). The two Bayesian Neural networks we deal with in this project Bohamiann and Numpyro BNN are similar regression models, but are infered using two different versions of the MCMC method, Hamiltonian Monte Carlo. As it will be revealed later (see result section) approximate inference might indeed be flawed and inexact.

Model	Predictive inference	Learning
GP	Exact $O(n^3)$	Emperical Bayes
SPN	Exact $O(E)$	EM $O(E)$
Gaussian Mixture Regression	Exact $O(K)$	EM
Bohamiann	Adaptive stochatic HMC	
Numpyro BNN	No U-Turn Sampler	

Table 5.1: Overview of inference methods applied on the statistical models used in this project. E is the number of edges in the SPN. n is the number of datapoints. $K \leq n$ is the number of mixture comonents. We will soon learn that for an SPN the number of mixture compenets is exponential larger than number of edges i.e. $E << K$. In theory MCMC methods samples from true the posterior distribution, and do not need any fitting/learning.

5.2 SPN

Sum-product networks are generative models, i.e. statistical models of the joint distribution $p(x, y)$. We need, however, a discriminative model for regression, i.e. a model of the conditional distribution $p(y|x)$. SPNs allow for exact inference of the joint distribution and any marginalized distribution. These combined queries is sufficient for the exact predictive posterior.

5.2.1 SPN - prediction

Prior to the inference of the predictive distribution, we assume that the SPN, S, is trained, i.e. trained leaf distributions $p_j(\cdot)$ for all leaf nodes, $j \in \mathcal{L}eaf(S) := \{j \in \mathcal{V}(S)|pa(j) = \emptyset\}$ and weights $w_{i,j}$ for the connections between every sum nodes $i \in \mathcal{S}$ and its children, $j \in ch(i)$.

The joint and the marginal distribution are evaluated in the following recursive way

---

Calculation of $p(x, y)$

Input: Fully trained SPN, with leaf distributions $p_i(\cdot)$ for $i \in \mathcal{L}eaf(S)$ and weigts $w_{i,j}$ for $(i, j) \in \{(i, j)|i \in \mathcal{S}um(S), j \in ch(i)\}$
function Eval(node i)
    if $i \in \mathcal{L}eaf(S)$ **then**
        return: $p_i(x, y)$ $\triangleright$ evaluate leaf distributions at point (x, y)
    if $i \in \mathcal{S}um(S)$ **then**
        return: $\sum_{j \in ch(i)} w_{i,j}\text{Eval}(j)$
    if $i \in \mathcal{P}rod(S)$ **then**
        return: $\prod_{j \in ch(i)} \text{Eval}(j)$
  $p(x) = \text{Eval(root)}$

Calculation of $p(x)$

Input: Fully trained SPN, with leaf distributions $p_i(\cdot)$ for all leaves i and weigts $w_{\cdot,\cdot}$.
function Eval(node i)
    if $i \in \mathcal{L}eaf(S)$ **then**
        if node handle x **then**
            return: $p_i(x, y)$ $\triangleright$ evaluate leaf distributions at point (x, y)
        else
            return: 1 $\triangleright$ set node equal 1 at point (x, y)
    if $i \in \mathcal{S}um(S)$ **then**
        return: $\sum_{j \in ch(i)} w_{i,j}\text{Eval}(j)$
    if $i \in \mathcal{P}rod(S)$ **then**
        return: $\prod_{j \in ch(i)} \text{Eval}(j)$
  $p(x) = \text{Eval(root)}$

So after doing two slightly different forward passes through the SPN, $p(x)$ and $p(x, y)$, using Bayes rule, we can combined the two queries into the conditional distribution:

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

The predictive distribution is found with a cost of just $O(E + E + 1) = O(E)$, where E is number of edges/connections in the SPN.

5.2.2 SPN - learning

It is not enouth to do predictive inference on a SPN, we also need to fit it on the data. It is possible interpret sum-product network as a large mixture model and therefore use expectation-maximization to train the model. We will introduce that idea now. The Paper [**SPN_EM**]... defines SPN as a mixture of all sub-networks of an SPN.

Definition 2 *A sub-network $\bar{S}_z$ of S is an SPN, which includes the root S and then includes nodes according to the following recursive scheme:*

Collection of sub-network S_z of S

---

    function Process(node i, S_z)
        if $i \in \mathcal{L}eaf(S)$ **then**
            return:
        if $i \in \mathcal{S}um(S)$ **then**
            $S_z = S_z.add(j \in ch(i))$ ▷ include one child of node i
            return: Process(j, S_z)
        if $i \in \mathcal{P}rod(S)$ **then**
            $S_z = S_z \cup \{j|j \in ch(i)\}$ ▷ include all childen of node i
            for $j \in ch(i)$ **do**
                return: Process(j, S_z)
        return: S_z
    S_z = Process(root,Ø)

So we see that at each sum node the number of different sub-networks multiplies with the number of children for that sum node. And thereby, the total number of sub-networks is

$$Z = \prod_{i \in \mathcal{S}um(S)} |ch(i)|$$

i.e. an exponential large amount of sub-networks. This is the amount of mixture components implicitly defined in an SPN. Denote the set of edges in the sub-network $\mathcal{E}(S_z)$. Now the we define a mixture coeficient, λ_z and component for each S_z as

$$\lambda_z := \prod_{(i,j) \in \mathcal{E}(S_z)} w_{i,j}, \qquad p_z(x,y|\theta) := \prod_{i \in \mathcal{L}(S_z)} p_i(x,y)$$

where $p_i(x,y)$ is the leaf distribution at leaf node i paramitised with θ. It can now be proven that the SPN can be interpreted as the following mixture model,

$$p(x,y|w,\theta) = \sum_{z=1}^{Z} \lambda_z(w)p_z(x,y|\theta)$$

i.e. by the weighted sum of all Z sub-networks. For convinience we define each sum component as $p(z,x,y|w,\theta) := \lambda_z(w)p_z(x,y|\theta)$. Evaluation of $p(x,y|w,\theta)$ will never be done as the sum over Z components, instead there is a proposition.

Proposition 2 *Consider a SPN, S, a sum node $q \in \mathcal{S}um(S)$ and a child $i \in ch(q)$, then the following relation holds,*

$$\sum_{z:(q,i) \in \mathcal{E}(S_z)} \lambda_z(w)p_z(x,y|\theta) = w_{i,q}\frac{\partial S}{\partial v(q)}v(i)$$

> **Background: Expectation-maximization EM**
> Expectation maximization is a convinient method for finding ML or MAP estimate of a latent

variable model. We consider a probibalistic model paramitised with θ,

$$p(\mathbf{X}, \mathbf{Z}|\theta)$$

where we denote all latent variables $\mathbf{Z}$, and observed variables $\mathbf{X}$. Our goal is to find the maximum of the likehood,

$$p(\mathbf{X}|\theta) = \int p(\mathbf{X}, \mathbf{Z}|\theta)\mu(d\mathbf{Z})$$

maximizating the likehood itself $p(\mathbf{X}|\theta)$ is assumed deficult but maximizating of the *complete-data* likehood $p(\mathbf{X}, \mathbf{Z}|\theta)$ is much easier.

The algorithm iterates over two steps, expecation step and a maximization step, defined in the following way for iteration t,

E-step Define the functional $Q(\theta, \theta^{(t)})$, to be the expected value of the complete-data log likehood (log likelihood function of θ), where the only random quantaty $\mathbf{Z}$ is assumed to follow a distribtuion with the density $p(\mathbf{Z}|\mathbf{X}, \theta^{(t)})$, i.e. the conditional distribution of $\mathbf{Z}$ given $\mathbf{X}$ and the current parameter point estimate $\theta^{(t)}$, i.e.

$$Q(\theta, \theta^{(t)}) := E_{p(\mathbf{Z}|\mathbf{X}, \theta^{(t)})}[\log p(\mathbf{X}, \mathbf{Z}|\theta)]$$

M-step Next we find the point estimate $\theta^{(t+1)}$ which maximizes $Q(\cdot|\theta^{(t)})$, i.e.

$$\theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)})$$

Proof that maximizing $Q(\cdot|\theta^{(t)})$, maximizes the likelihood $p(\mathbf{X}|\theta)$. From $p(\mathbf{X}|\theta) = \frac{p(\mathbf{X}, \mathbf{Z})}{p(\mathbf{X})}$ we can write

$$\log p(\mathbf{X}|\theta) = \log p(\mathbf{X}, \mathbf{Z}) - \log p(\mathbf{Z}|\mathbf{X}, \theta)$$

Now, taking the expecation of the above w.r.t. $p(\mathbf{Z}|\mathbf{X}, \theta^{(t)})$, yields,

$$\log p(\mathbf{X}|\theta) = E_{p(\mathbf{Z}|\mathbf{X}, \theta^{(t)})}[\log p(\mathbf{X}, \mathbf{Z}|\theta)] - E_{p(\mathbf{Z}|\mathbf{X}, \theta^{(t)})}[\log p(\mathbf{Z}|\mathbf{X}, \theta)]$$
$$= Q(\theta, \theta^{(t)}) + E_1[\log p(\mathbf{Z}|\mathbf{X}, \theta)]$$

Since the above equation holds for any θ, it also holds for $\theta^{(t)}$ now we have,

$$\log p(\mathbf{X}|\theta^{(t)}) = Q(\theta^{(t)}, \theta^{(t)}) + E_1[\log p(\mathbf{Z}|\mathbf{X}, \theta)]$$

combining the two equations, we get,

$$\log p(\mathbf{X}|\theta) - \log p(\mathbf{X}|\theta^{(t)}) = Q(\theta, \theta^{(t)}) - Q(\theta^{(t)}, \theta^{(t)}) + E_1[\log p(\mathbf{Z}|\mathbf{X}, \theta)] - E_1[\log p(\mathbf{Z}|\mathbf{X}, \theta^{(t)})]$$

From Gibb's inequality we have that $E_1[\log p(\mathbf{Z}|\mathbf{X}, \theta^{(t)})] \leq E_1[\log p(\mathbf{Z}|\mathbf{X}, \theta)]$ where equality only holds for $\theta^{(t)} = \theta$, so we have

$$\log p(\mathbf{X}|\theta) - \log p(\mathbf{X}|\theta^{(t)}) \geq Q(\theta, \theta^{(t)}) - Q(\theta^{(t)}, \theta^{(t)})$$

so choosing θ, which improves $Q(\cdot, \theta^{(t)})$ $\log p(\mathbf{X}|\theta)$ has to improve as least as much.

then we can marginalise over z in order to recover $p(x)$,

$$p(\mathbf{x}|\pi) = \sum_{z=1}^{Z} p(z, \mathbf{x}|\pi)$$

assuming iid data, then the complete likehood can be decompose as the product

$$p(z, \mathbf{x}|\pi) = \prod_{i=1}^{n} p(z, \mathbf{x}_i|\pi)$$

We wil for convinience transform the likelihood using a log transform, as it will not influence the maximum.

$$\log p(\mathbf{x}|\pi) = \sum_{z=1}^{Z} \sum_{i=1}^{n} \log p(z, \mathbf{x}_i|\pi)$$

and a normal evaluation of $p(x, y|w_{old}, \theta_{old})$ combined in Bayes rule we obtain

$$p(z|x, y, w_{old}, \theta_{old}) = \frac{p(z, x, y|w_{old}, \theta_{old})}{p(x, y|w_{old}, \theta_{old})} = \frac{\lambda_z(w_{old})p_z(x, y|\theta_{old})}{p(x, y|w_{old}, \theta_{old})}$$

and we have the expecation for the EM-algorithm,

$$Q(\pi, \pi_{old}) = \sum_{n=1}^{N} \sum_{z=1}^{Z} p(z|xy_n, \pi_{old}) \ln p(z, xy_n|\pi)$$

Her er en titel

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5.3 Gaussian Mixture Regression

The Gaussian mixture is a generative model of the joint probability of x and y given as,

$$p(x, y) = \sum_{k=1}^{K} \pi^{(k)} \mathcal{N}(x, y|\mu^{(k)}, \Sigma^{(k)}), \qquad \mu = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}, \ \Sigma = \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix}$$

This is trained using the EM algorithm. We will now show how the conditial is calculated exact.

5.3.1 GMR - prediction

We need the conditional distribution of the Gaussian mixture in order to get the predictive distribution. We will now formulate the conditial distribution in terms of conditional and marginals of the individual mixture components. First of all the marginal distribution $p(x)$ of the mixture is given as, How??!

$$p(x) = \sum_{k=1}^{K} \mathcal{N}(x|\mu_x^{(k)}, \Sigma_{xx}^{(k)})$$

next the joint distribution can be decomposed with the probability chain rule,

$$p(x, y) = p(x)p(y|x)$$
$$\implies \quad \mathcal{N}(x, y|\mu, \Sigma) = \mathcal{N}(x|\mu_x, \Sigma_{xx})\mathcal{N}(y|\mu_{y|x}, \Sigma_{y|x})$$

And we can formulate the conditial in terms of individual multivariate Gaussians,

$$p(y|x) = \frac{p(y, x)}{p(x)} \tag{5.1}$$

$$= \sum_{k=1}^{K} \frac{\pi^{(k)}}{p(x)} \mathcal{N}(x, y|\mu^{(k)}, \Sigma^{(k)}) \tag{5.2}$$

$$= \sum_{k=1}^{K} \frac{\pi^{(k)} \mathcal{N}(x|\mu_x^{(k)}, \Sigma_{xx}^{(k)})}{p(x)} \mathcal{N}(y|\mu_{y|x}^{(k)}, \Sigma_{y|x}^{(k)}) \tag{5.3}$$

$$= \sum_{k=1}^{K} \pi_{y|x}^{(k)} p(y|x, \mu_{y|x}^{(k)}, \Sigma_{y|x}^{(k)}) \tag{5.4}$$

where $\pi_{y|x}^{(k)} := \frac{\pi^{(k)} \mathcal{N}(x|\mu_x^{(k)}, \Sigma_{xx}^{(k)})}{\sum_{i=1}^{K} \mathcal{N}(x|\mu_x^{(i)}, \Sigma_{xx}^{(i)})}$. So we see that the conditonal of a Gaussian mixture model is again a Gaussian mixture model.

> **Background: Conditional og multivariate Gaussian**
> The conditional distribution is defined as <ref bishop>
>
> $$p(y|x, \mu, \Sigma) = \mathcal{N}(y|\mu_{y|x}, \Sigma_{y|x}) \qquad \mu = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}, \ \Sigma = \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix}$$
>
> where
>
> $$\mu_{y|x} = \mu_y + \Sigma_{yx}\Sigma_{xx}^{-1}(x - \mu_x) \tag{5.5}$$
> $$\Sigma_{y|x} = \Sigma_{yy} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy} \tag{5.6}$$

5.3.2 GMR - Leaning

EM-algorithm, classic example.

5.4 Gaussian Process Regression

We now show how the preditive distribution is calculated exact for Gaussian Processes, i.e.

$$p(y|x, \mathcal{D}) = \int \mathcal{N}(y|f(x), \sigma^2)p(f(x)|\mathcal{D})df(x) \tag{5.7}$$

we will soon see that $p(f(x)|\mathcal{D}) = \mathcal{N}(f(x)|.., ...)$ and and thereby that we have a marginal Gaussian distribution for $f(x)$ and a conditional Gaussian distribution of y given $f(x)$, giving us the marginalized distribtuion, $p(y|x, \mathcal{D})$, using formulars (5.8).

> **Background: Trick with normal distributions [from Bishops book?]**
> Given a marginal Gaussian distribution of x and a conditional Gaussian distribution of y given x of the form,
>
> $$p(x) = \mathcal{N}(x|\mu, \Lambda^{-1})$$
> $$p(y|x) = \mathcal{N}(x|Ax + b, L^{-1})$$
>
> then the marginal distribution of y and the conditional distribution of x given y have the form,
>
> $$p(y) = \mathcal{N}(y|A\mu + b, L^{-1} + A\Lambda^{-1}A^T) \tag{5.8}$$
> $$p(x|y) = \mathcal{N}(x|\Gamma\mu + \Gamma[A^T L(y - b)], \Gamma) \tag{5.9}$$
> $$\Gamma := (\Lambda + A^T LA)^{-1} \tag{5.10}$$

Posterior function

Recall we assume $\mathbf{f} = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))$ is the parameters in our model, therefore we call $p(\mathbf{f}|\mathcal{D})$ the posterior distribution. However, what is of real interest is the function values on unobserved locations, thereby we extend $\mathbf{f}$ to be a function, i.e. an infinitely dimentional vector. We call this quantaty *the posterior function*

$$p(f(\cdot)|\mathcal{D}) = \int p(f(\cdot)|\mathbf{x}, \mathbf{f})p(\mathbf{f}|\mathcal{D})d\mathbf{f}. \tag{5.11}$$

Prior we assume that the function takes values accoring to

$$p(\mathbf{f}|\mathbf{x}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, c(\mathbf{x}, \mathbf{x}))$$

where the covariance is defined at kernel evaluation for each pair of $\mathbf{x}$, where $c(\cdot, \cdot)$ is a covariance function, chosen to be the Matérn covariance function,

$$c(\mathbf{x}, \mathbf{x}) = \begin{bmatrix} c(x_1, x_1) & \ldots & c(x_1, x_n) \\ \vdots & \ddots & \\ c(x_n, x_1) & \ldots & c(x_n, x_n) \end{bmatrix} \qquad c(x, y) := Matern(x, y)...$$

We now calculate the first term in the integral (5.11), $p(f(\cdot)|\mathbf{x}, \mathbf{f})$ using that we have the joint prior distribution,

$$p(f(\cdot), \mathbf{f}|\mathbf{x}) = \mathcal{N}\left(\begin{bmatrix} f(\cdot) \\ \mathbf{f} \end{bmatrix} \middle| \begin{bmatrix} 0 \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} c(\cdot, \cdot) & c(\cdot, \mathbf{x}) \\ c(\mathbf{x}, \cdot) & c(\mathbf{x}, \mathbf{x}) \end{bmatrix}\right) \tag{5.12}$$

And the conditonal of a joint Gaussian is given using <ref>

$$p(f(\cdot)|\mathbf{x}, \mathbf{f}) = \mathcal{N}(f(\cdot)|c(\cdot, \cdot)^{-1}c(\cdot, \mathbf{x})\mathbf{f}, c(\cdot, \cdot)^{-1})$$

Next we calculate the last term in the integral (5.11), $p(\mathbf{f}|\mathcal{D})$, i.e. the posterior distribution. Assuming iid data, i.e. $p(y_1, \ldots, y_n|x_1, \ldots, x_n, \mathbf{f}) = \prod_{i=1}^n p(y_i|x_i, \mathbf{f}_i)$ and that the likelihood is Gaussian with mean $\mathbf{f}$ and variance $\sigma^2 I_n$.

$$p(\mathbf{f}|\mathcal{D}) \propto p(\mathbf{f}|x) \prod_{i=1}^{n} p(y_i|x_i, \mathbf{f}_i)$$

$$= \mathcal{N}(\mathbf{f}|\mathbf{0}, c(\mathbf{x}, \mathbf{x})) \prod_{i=1}^{n} \mathcal{N}(y|\mathbf{f}_i, \sigma^2)$$

$$= \mathcal{N}(\mathbf{f}|\mathbf{0}, c(\mathbf{x}, \mathbf{x})) \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I_n)$$

now from <ref> we have that the posterior is the following Gaussian:

$$p(\mathbf{f}|\mathcal{D}) = \mathcal{N}(\mathbf{f}|M^{-1}\sigma^{-2}\mathbf{y}, M^{-1}) \quad M := c(\mathbf{x}, \mathbf{x})^{-1} + \sigma^{-2} I_n$$

Now we found that both term in the integral (5.11), and they are related such that it is possible to use (5.8) for arriving at (we define $A := c(\cdot, \cdot)^{-1} c(\cdot, \mathbf{x})$),

$$p(f(\cdot)|\mathcal{D}) = \mathcal{N}(f(\cdot)|AM^{-1}\sigma^{-2}\mathbf{y}, c(\cdot, \cdot)^{-1} + AM^{-1}A^T)$$

Finally we found that both terms in the integral (5.7) also is related in a simlar way, and we use (5.8), again to arrive at the predictive distribtuion,

$$p(y_*|x_*, \mathcal{D}) = \mathcal{N}(y_*|AM^{-1}\sigma^{-2}\mathbf{y}, c(x_*, x_*)^{-1} + AM^{-1}A^T + \sigma^2)$$

Some questions about a naive approach..!

Learning - Emperical bayes inference
Anther inference which is done is then optimizing the hyper parameters using emperical bayes i.e. the variance and length scale for the kernel. Here we optimize the marginalized likelihood function

$$p(y_1, \ldots, y_n | x_1, \ldots, x_n, \theta) = -\frac{1}{2}[(y - \mu)^T (\Sigma + N)^{-1}(y - \mu) + \log|\Sigma + N| + n \log 2\pi]$$

<and how to get to there?>

Model assessment becomes trivial in light of the model posterior if we simply establish preferences over models according to their posterior probability. When using the uniform model prior (4.6) the model posterior is proportional to the marginal likelihood alone, which can be then used directly for model assessment. ??! Forstår ikke

5.5 Deep Network Global Optimization - ?
?? Kernel regression :-)) Should I not work on this?

5.6 Bayesian Neural Networks
Bohamiann and numpyro-BNN are examples of probabilistic models with intractable inference. The predictive density is given as,

$$p(y_*|x_*, \mathcal{D}) = \int p(y_*|x, \theta) p(\theta|\mathcal{D}) d\theta$$

$$\approx \frac{1}{K} \sum_{k=1}^{K} p(y_*|x, \theta^{(k)})$$

where the first integral is intractable as θ can live in a highly dimensional space, second the approximation sign is true, since we can aproximate the integral with monte carlo sampling: $\theta^{(k)}$ are iid samples from the posterior distribution, $\theta^{(k)} \sim p(\theta|\mathcal{D})$. We can get samples from the posterior distriution

Assuming we have a number of iid samples, $\theta^{(1)}, \ldots, \theta^{(K)}$ drawn from the distribution $p(x)$, then the following appriximation

$$E[f(x)] \approx \frac{1}{K} \sum_{k=1}^{K} f(x^{(k)}) =: \Theta_K(f)$$

holds accoring to the law of large numbers in fact

$$E[f(x)] = \lim_{K \to \infty} \Theta_K(f)$$

and the central limit theorem, <OBS refere!>

$$p(\hat{\Theta}) \approx \mathcal{N}(\hat{\Theta}|\mu_f, \frac{\sigma_f^2}{K})$$

which ensures that the variance of the unbiased estimator of the expecation decreases with number of samples, K. Left is to sample the iid samples from the distribution $p(x)$

Posterior samples

For both models the joint distribution $p(\mathcal{D}, \theta)$ is available, but calulating the posterior distribution requires the marginalized likehood, $p(\mathcal{D}) = \int_{\theta} p(\mathcal{D}, \theta)$. This integral is often intractable since the space of θ typically is abnomous - so not even nummerical apprixmations of the intergral is tractable. From Bayes rule, we have the equality,

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}, \theta)}{p(\mathcal{D})} \propto p(\mathcal{D}, \theta),$$

where the propotional sign is true, since $p(\theta|\mathcal{D})$ is a function of θ. Knowing the $p(\mathcal{D}, \theta)$ joint distribution thereby allow for using Markov chain Monte Carlo for sampling from the posterior distribution.

We can conviniently use MCMC for sampling from a probability density $p(x)$, with only the knowledge of a propotional/unnormalised density $\hat{p}(x) \geq 0$ i.e

$$\hat{p}(x) = c \cdot p(x) \qquad c = \int \hat{p}(x) dx,$$

where $\int \hat{p}(x) dx$ is a possible intractable integral. An ergodic Markov chain/process is constructed, such that its stationary distribution is exactly $p(x)$, but only with the knowledge of $\hat{p}(x)$.

The most simple MCMC method is the Metropolis-Hasting algorithm. At iteration n we have a sample x_n,

1. Propose $\hat{x}$ from a proposal density $q(x_n, \cdot)$

2. Compute accptance probability

$$\alpha(x_n, \hat{x}) = \min \left(1, \frac{p(\hat{x})}{p(x_n)} \frac{q(\hat{x}, x_n)}{q(x_n, \hat{x})} \right)$$

3. Set the next sample

$$x_{n+1} = \begin{cases} \hat{x} & \text{with probability } \alpha(x_n, \hat{x}) \\ x_n & \text{with probability } 1 - \alpha(x_n, \hat{x}) \end{cases}$$

note that $\alpha(x_n, \hat{x})$ requires $p(x)$, but since the algorithm only requires the fraction $\frac{p(\hat{x})}{p(x_n)} = \frac{p(\hat{x}) \cdot c}{p(x_n) \cdot c} = \frac{\hat{p}(\hat{x})}{\hat{p}(x_n)}$ we only need $\hat{p}$.

Proof: Assuming discrete states, the transition probability between the states are given as,

$$p(x \to y) = \begin{cases} q(x, y)\alpha(x, y) & \text{if } x \neq y \\ q(x, x) + \sum_{z \neq x} q(x, z)(1 - \alpha(x, z)) & \text{if } x = y \end{cases}$$

Now, let us look at the so-called *detailed balance* relation, i.e. that if we are sampling from the stationary density we stay there at the next state. Assume $x \neq y$,

$$p(x)p(x \to y) = p(x)q(x, y)\alpha(x, y)$$
$$= p(x)q(x, y) \min\left(1, \frac{p(\hat{x})}{p(x_n)} \frac{q(\hat{x}, x_n)}{q(x_n, \hat{x})}\right)$$
$$= \min(p(x)q(x, y), p(y)q(y, x))$$

Observing that the right hand side yields symmetric result in x and y, therefore we obtain,

$$p(x)p(x \to y) = p(y)p(y \to x)$$

and summing over x on both sides yields,

$$\sum_x p(x)p(x \to y) = p(y) \sum_x p(y \to x) \tag{5.13}$$
$$\implies \quad p(y) = \sum_x p(x)p(x \to y) \tag{5.14}$$

similar conclusion will be obtained for $x = y$, all in all this reveals that $p(x)$ is in fact invariant for the chain $\{x_1, \ldots, x_n\}$ and thereby that MH is a MCMC algorithm.

HM with random walk transition is very simple and it comes with some serious disadvantages: slow convergence speed, might stay in the same region for a long time and produces highly correlated sampels. We can do better by replacing the random walk with gradient-guided movements and intepretate the probability landscape as a physical system.

Example: HMC
The golden standard in MCMC is the Hamilton monte carlo, which exploits arguments from classical mechanics around the Hamiltonian equations. This method leads to more efficient sampling as the Hamiltonian intepretation allows the system to take regions with high probability mass into acound - this is optained using gradient of the probability landscape. $\frac{-\partial E(x)}{\partial x}$

We define PDF

$$p(x) = \frac{1}{Z_E} \exp(-E(x)),$$

where $E(x)$ is interpretted as the systems potential energy. Now, an latent vector q is introduced in order to represent the momentum of the system, which gives us the kinetic energy of the

system.

$$K(q) = \frac{1}{2} \sum_{i=1}^{l} q_i^2$$

Giving the Hamilton function and its coresponing distribution

$$H(x, q) = E(x) + K(q)$$

and

$$p(x, q) = \frac{1}{Z_H} \exp(-H(x, q)) \tag{5.15}$$

$$= \frac{1}{Z_E} \exp(-E(x)) \frac{1}{Z_K} \exp(-K(x)) \tag{5.16}$$

$$= p(x)p(q) \tag{5.17}$$

The desired distribution $p(x)$ is found as the marginal of $p(x, q)$

since some intuition is now established around Hamiltonian Monte Carlo, we look a bit on the two versions used in Numpyro-BNN and Bohamiann,

5.6.1 No U-Turn sampling

othen the physical simulation in HMC goes forth and back the same path, and we risk getting bad samples. No U-turn (NUTS) sampling avoid this.

5.6.2 Adaptive stochatic HMC

...

5.7   Appendix - SPN

Normalization of SPN

Calculation of Z

Input: node i
function Eval(node i)
    if i is leaf **then** $\triangleright$ leaf node
        return: 1 $\triangleright$ set node equal 1 at point (x, y)
    if $i \in \mathcal{S}$ **then**
        return: $\sum_{j \in ch(i)} w_{i,j} \text{Eval}(j)$
    if $i \in \mathcal{P}$ **then**
        return: $\prod_{j \in ch(i)} \text{Eval}(j)$
  $Z = \text{Eval(root node)}$

Investigation of Deep Probibalistic Surrogate-models in Bayesian Optimization

6 Results

<reproducer resultater fra Arayns thesis> Egne forsøg med SPN og mixture regression

6.0.1 regression benchmark
We will benchmark our different regression models againt a simple emperical mean and emperical std. normal distribution benchmark,

$$p(y|x\mathcal{D}) = \mathcal{N}(y|\bar{\mathbf{y}}, \bar{\sigma}^2(\mathbf{y}))$$

where $\bar{\mathbf{y}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{y}_i$ and $\bar{\sigma}^2(\mathbf{y})) = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{y}_i - \bar{\mathbf{y}})^2$ this is however not a good model for Bayesian optimization, as it will not provide a new candidate point, as all points are equally good.

7 Colours

The design guide define 3 primary colours (dtured, white and black) and 10 secondary colours https://www.designguide.dtu.dk/#stnd-colours. Below are codes for the various colour modes. RGB is used for web and Office Programmes. CMYK is used for print. HTML is used for HTML-coding. If you know anything about colour codes you might notice that the RGB codes are ranging from 0-1 instead of the usual 0-255.

color	rgb	cmyk	HTML
dtured	0.77 0 0.05	0 0.91 0.72 0.23	C4000D
white	1 1 1	0 0 0 0	FFFFFF
black	0 0 0	0 0 0 1	000000
blue	0.12 0.24 1	0.88 0.76 0 0	1F3DFF
brightgreen	0.31 1 0.34	0.69 0 0.66 0	4FFF57
navyblue	0 0 0.4	1 0.9 0 0.6	000066
yellow	0.95 0.83 0.18	0.05 0.17 0.82 0	F2D42E
orange	1 0.35 0.14	0 0.65 0.86 0	FF5924
pink	1 0.65 0.74	0 0.35 0.26 0	FFA6BD
red	1 0.14 0.35	0 0.86 0.65 0	FF2459
green	0 0.78 0	0.89 0.05 1 0.17	00C700
purple	0.33 0.04 1	0.67 0.96 0 0	540AFF

The default colour mode for this template is cmyk. The current colour model is cmyk which is also illustrated by the underlined numbers in the colour test table above. If you which to change the colour model to rgb go to Setup/Settings.tex and change `targetcolourmodel` to rgb. In Setup/Settings.tex it is also possible to change the background colour of the front and back page. The colours are primarily used for diagrams (the plotcyclelist DTU) and the front and back page.

Lighter colours can be achieved as written in the LATEX code below. For example to get a tint of 50% you would write colourname!50.

Normal dtured   80% dtured   70% dtured   60% dtured   50% dtured

For more information about colours in LATEX read the `xcolor` manual.

hej

8 Examples of figures, tables, equations and listings

In the following a bunch of examples of figures and tables have been made. There are advantages to using `tikZ` diagrams over excel diagrams. 1) the font and font size perfectly matches the document 2) the styling and colours are pre-defined to follow the design guide 3) the plots uses vector graphics which reduces the file size, reduces the compile time and looks sharp when zooming in. The possibilities are endless, look at the `pgfplots` gallery for inspiration: http://pgfplots.sourceforge.net/gallery.html. However there are still cases where I would recommend to insert a plot as a picture. For example if the plot contains a lot of data: a line graph with 1000 points takes a long time to compile.

Some tips if you want good looking diagrams or graphs which will be inserted as pictures (e.g. in a figure environment with \includegraphics): The main font is Arial. Use DTU colours as described in chapter 7. Use high quality pictures. Try to scale the diagram (picture) so the text size of the axis legends match the text size in this document.

Remember to change the label of your figures so there are no duplicate labels. A label should be placed below a caption or after a heading (fx after a \chapter).
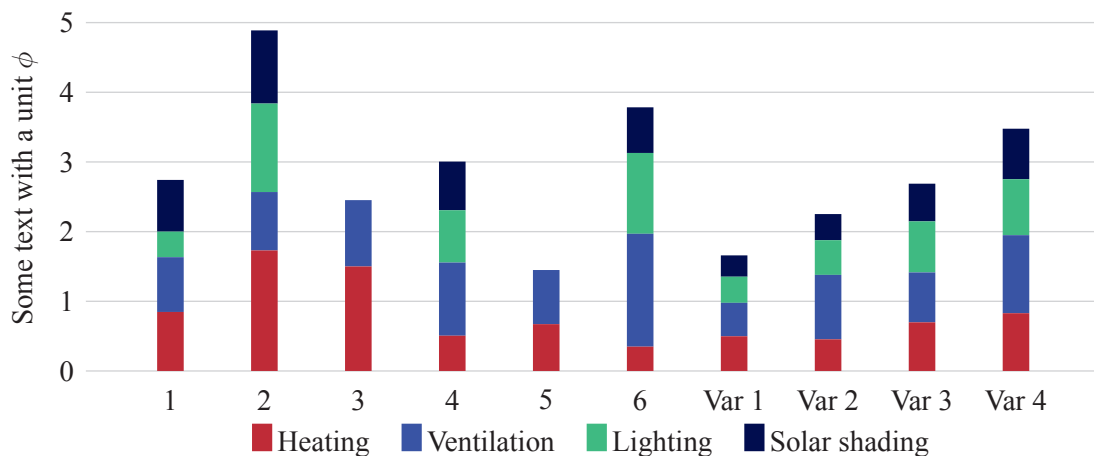
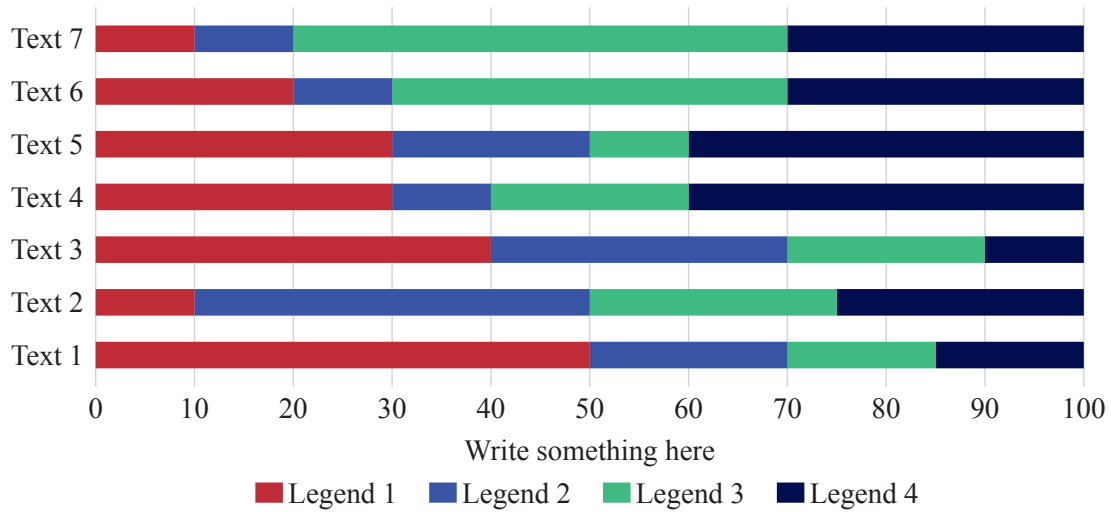## 8.1 Graphs and charts

Figure 8.1: Stacked column chart
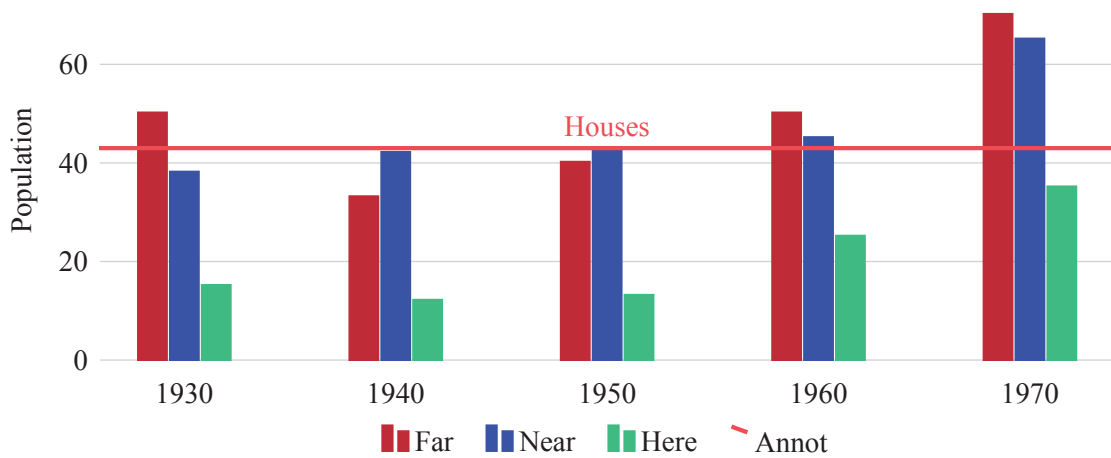
Figure 8.2: Stacked bar chart

Figure 8.3: Grouped column chart

Figure 8.4: Line graph

Investigation of Deep Probibalistic Surrogate-models in Bayesian Optimization
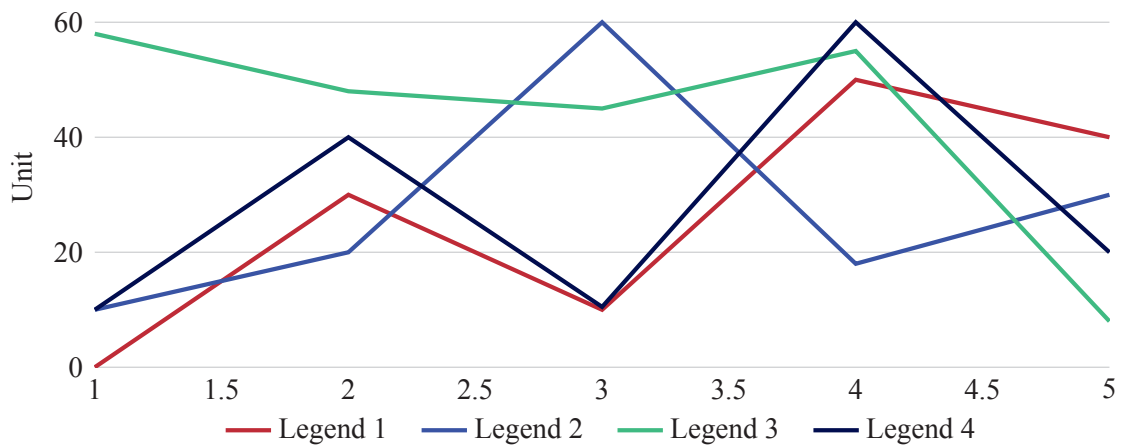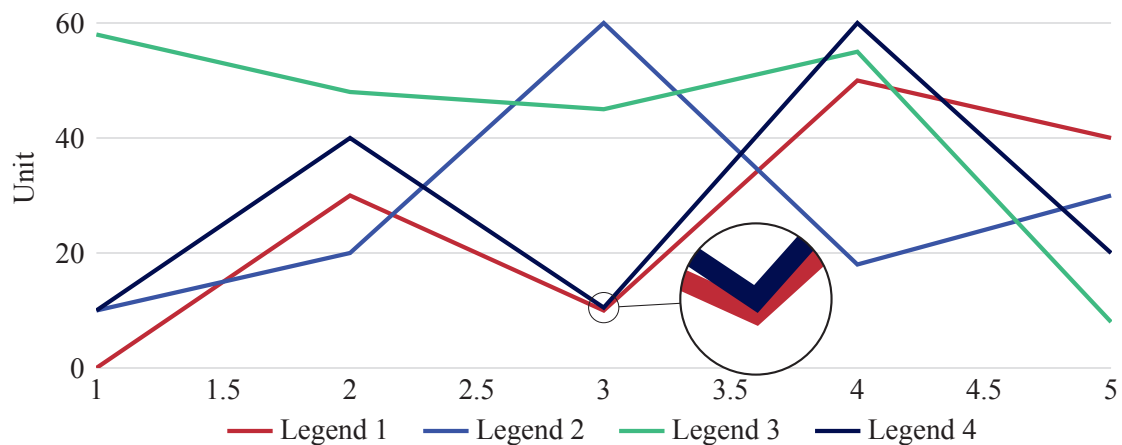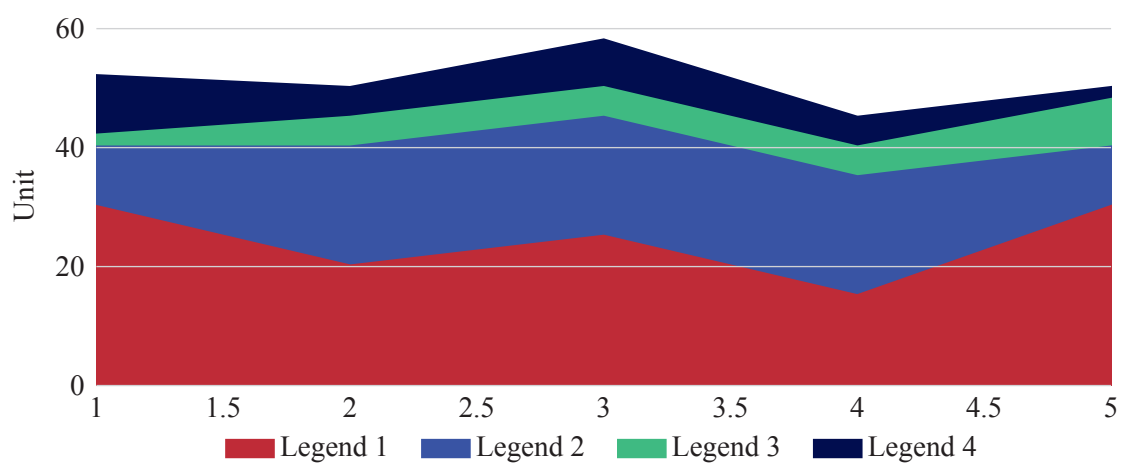
Figure 8.5: Line graph with magnifying glass

Figure 8.6: Area graph

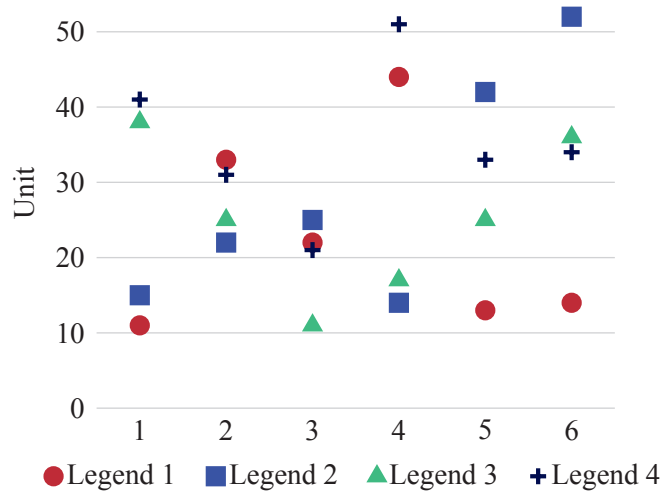Figure 8.7: Scatter plot
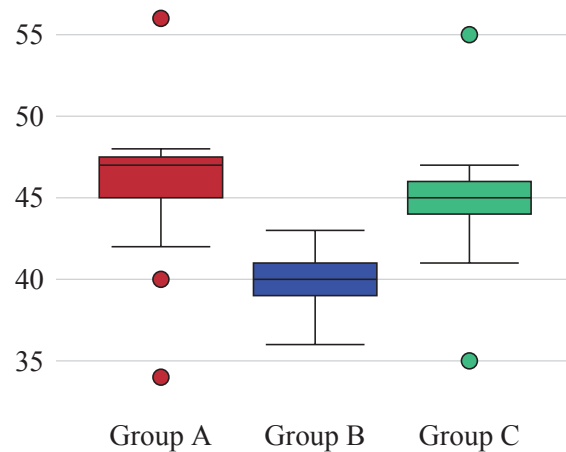
Figure 8.8: Boxplot

8.2 Tables and figures

Table 8.1: This is a `booktabs` table. Go to http://www.tablesgenerator.com/ and use the book-tabs table style

	Item	
Animal	Description	Price($)
Gnat	per gram	13.65
	each	0.01
Gnu	stuffed	92.50
Emu	stuffed	33.33
Armadillo	frozen	8.99

`Booktabs` tables don't use any vertical lines. Only horizontal lines are used. Table 8.1 begins with a \toprule, ends with a \bottomrule with \midrule in between. The table has 3 columns formatted as @{}llS@{}. @{} is cropping the horizontal lines of the table to fit the content (removes column spacing at the left and right edges). l aligns the column to the left and S aligns the column according to the decimal point (`siunitx` package). You can of course also use r to align right or c to center the contents of the column.

Table 8.2: Wrongly formatted table

	Voltage V	Current A	Power W
Transformer input	234.4	0.50	117.4
Transformer output	25.86	2.72	70.3
Efficiency			60%

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Table 8.3: Correctly formatted table

	Voltage V	Current A	Power W
Transformer input	234.4	0.50	117.4
Transformer output	25.86	2.72	70.3
Efficiency			60 %

Table 8.2 and table 8.3 have the same comtents but there are some subtle differences in formatting which makes table 8.3 the superior table of the two. The most obvious change is removing the midrule between the transformer input and output rows. The effcency row is the odd man out and a midrule has been used to emphasise the difference between the transformer rows and the efficiency row. The delimiters in the voltage, current and power columns are aligned. The horizontal lines (rules) fits to the content and instead of protruding. The spacing between 60 and the percentage sign is correctly adjusted.

Figure 8.9: Just a normal figure

(a) A subfigure

(b) A subfigure

Figure 8.10: A figure with two subfigures

(a) A subfigure

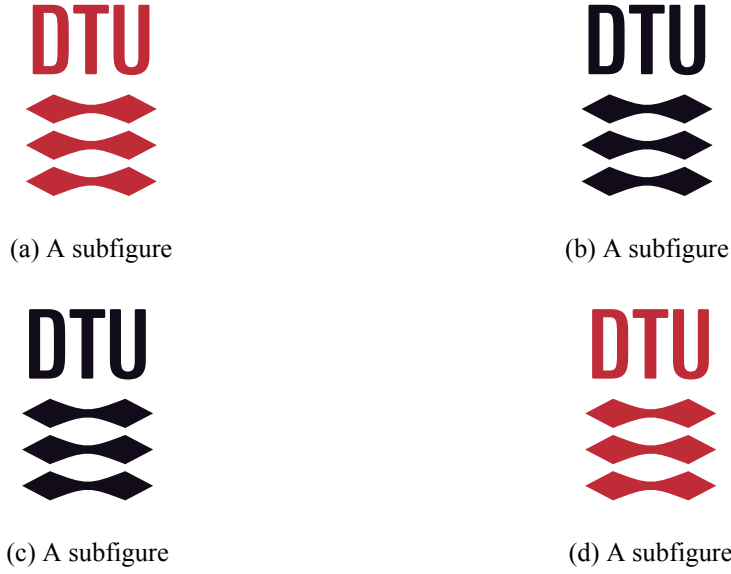(b) A subfigure

(c) A subfigure

(d) A subfigure

Figure 8.11: A figure with four subfigures

Referring to the figure as a whole fig. 8.11 or to an individual sub figure fig. 8.11a is done the normal way with `\cref{}` commands.

8.3 Equations

In-line math is easy. Anything surrounded by dollar signs becomes a math field. Here is an example: $f(x) = 2x - 1$. Also anything inside the "\begin{equation}" and "\end{equation}" environment is also a math field. Examples are shown below.

All equations use the default latex font. Some might say it looks weird with a serif font for equations and a sans-serif font for the body text. However, it is very unpractical to change the math font in latex which is the exactly the reason why this has not been done. One benefit of the serif style math font is the clear distinction between symbols (variables) and units.

On the subject of units, those are all taken care of by the `\siunitx` package. Whenever there is a number followed by a unit one should write \SI{number}{unit}. Note this command is case sensitive. If a unit should follow a variable use the command \si{unit} (also case sensitive).
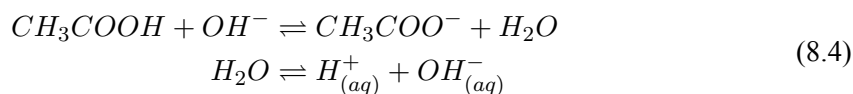
The ideal gas law is shown in eq. (8.1).

$$p \cdot V = n \cdot R \cdot T \tag{8.1}$$

$$\frac{\partial}{\partial t} \int_0^\delta U \, dy = -\delta \frac{1}{\rho} \frac{\partial P}{\partial x} - U_f(t)^2 \tag{8.2}$$

$$d_{step} = \sqrt{\frac{\delta}{\frac{dw}{dp_v}} \cdot t} = \sqrt{\frac{1.0 \times 10^{-11} \, \text{kg}/(\text{m s Pa})}{\frac{5.4 \, \text{kg/m}^3}{233.82 \, \text{Pa}}} \cdot 7200 \, \text{s}} = 0.001\,766 \, \text{m} = 1.766 \, \text{mm} \tag{8.3}$$

$$x = \mathbf{x}, \mathbf{x}, x, x_{1_{2_{3_4}}}^{1^{2^{3^4}}} \cdot hello * \text{hello world} \cdot \text{equation without number}$$

Notice how the `aligned` environment can be used to align the equilibrium arrows in eq. (8.4). Only one equation number is generated using this method. Alternatively if you want an equation number for each line see eqs. (8.5) to (8.6).

$$
\begin{aligned}
CH_3COOH + OH^- &\rightleftharpoons CH_3COO^- + H_2O \\
H_2O &\rightleftharpoons H^+_{(aq)} + OH^-_{(aq)}
\end{aligned}
\tag{8.4}
$$

$$
f(x) = 1 + x - 3x^2
\tag{8.5}
$$

$$
g(x) + y = 3x - \frac{1}{2}x^3
\tag{8.6}
$$

8.4 Listings (code)

Listing 8.1 is a nicely formatted block of code. A listing will automatically continue on the next page if it encounters a page break. Many different programming languages can be highlighted. Check the `listings` package documentation for a list of supported programming languages.

```
1  %% Monte Carlo simulation, estimation of pi
2  m=1E7;
3
4  x=rand(m,1);
5  y=rand(m,1);
6
7  g = x.^2+y.^2-1;
8
9  %dots outside
10 Pf = sum((g)<=0)/m
11
12 pi = 4*Pf
```

Listing 8.1: Monte Carlo simulation to estimate the value of π

A   Title

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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