Deep Learning

Lecture 8: Uncertainty

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Today

How to model uncertainty in deep learning?

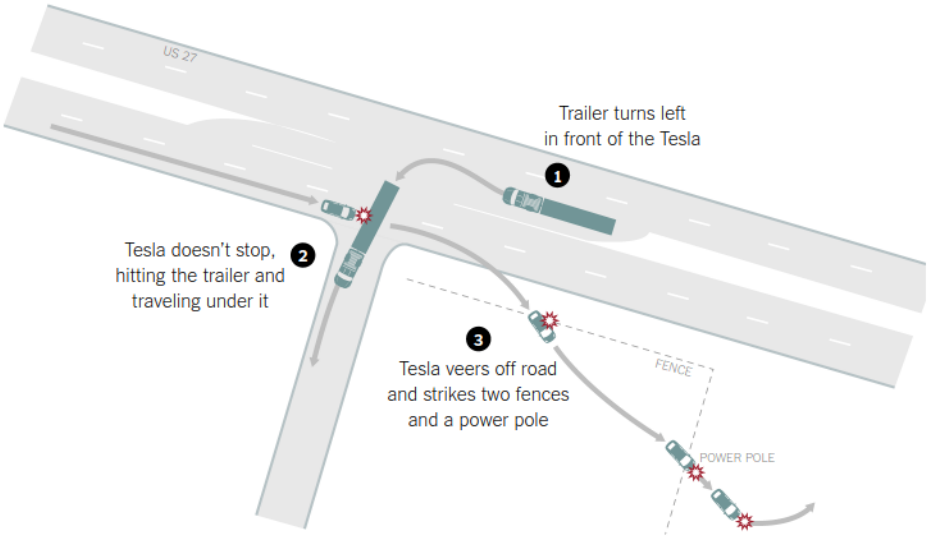
- Uncertainty
- Aleatoric uncertainty
- Epistemic uncertainty

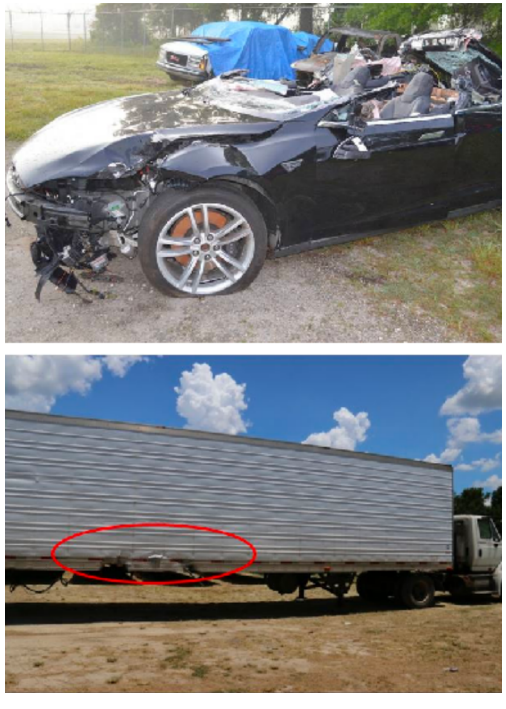
*"Every time a scientific paper presents a bit of data, it's accompanied by an **error bar** – a quiet but insistent reminder that no knowledge is complete or perfect. It's a **calibration of how much we trust what we think we know**." — Carl Sagan.*

Uncertainty

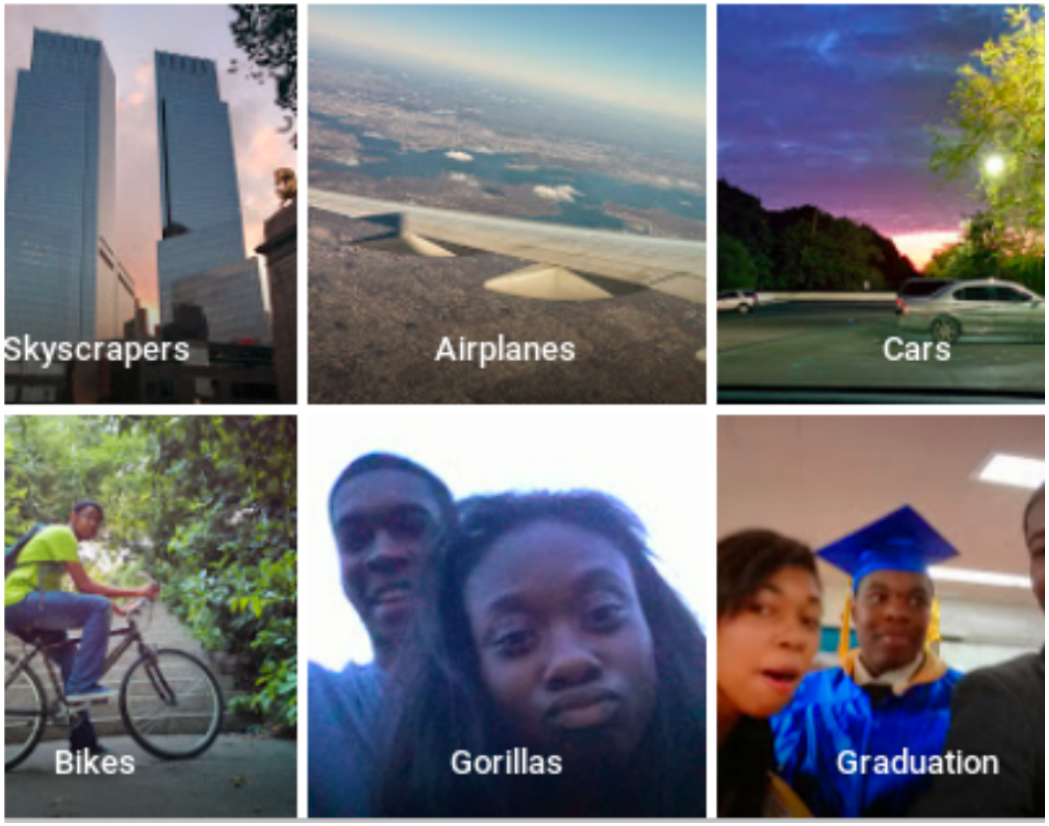
Motivation

In May 2016, there was the first fatality from an assisted driving system, caused by the perception system confusing the white side of a trailer for bright sky.





Credits: Kendall and Gal, What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision?, 2017.



An image classification system erroneously identifies two African Americans as gorillas, raising concerns of racial discrimination.

Credits: Kendall and Gal, What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision?, 2017.

If both these algorithms were able to assign a high level of uncertainty to their erroneous predictions, then the system may have been able to make better decisions, and likely avoid disaster.

Credits: Kendall and Gal, What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision?, 2017.

Types of uncertainty

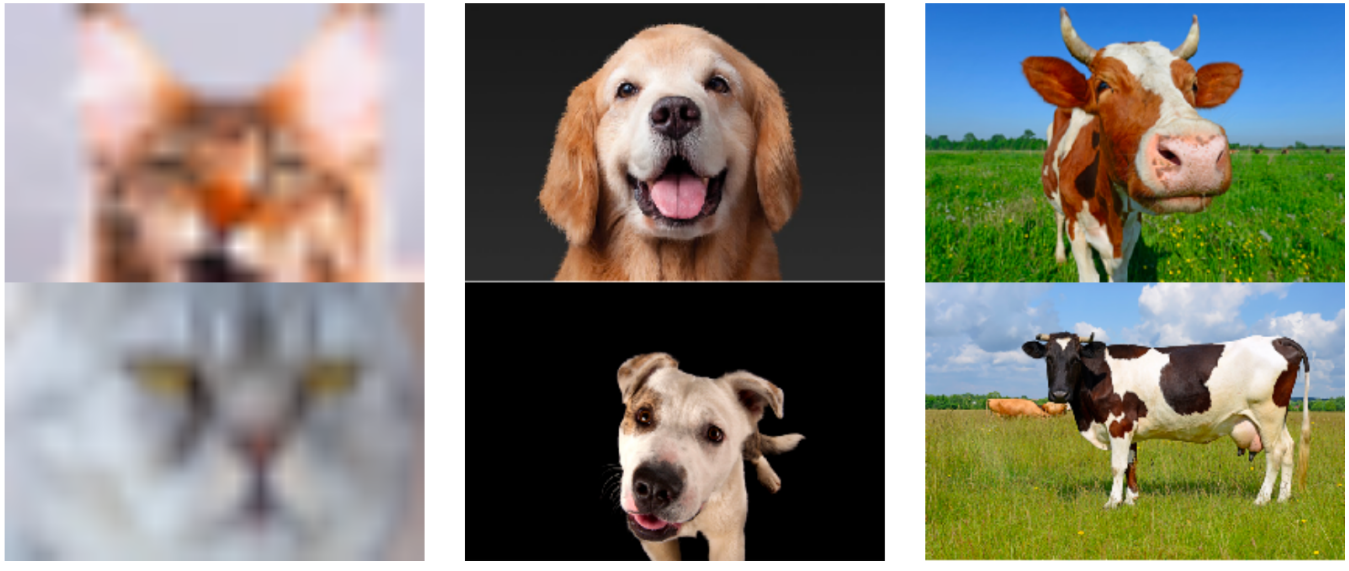
Case 1

Let us consider a neural network model trained with several pictures of dog breeds.

- We ask the model to decide on a dog breed using a photo of a cat.
- What would you want the model to do?

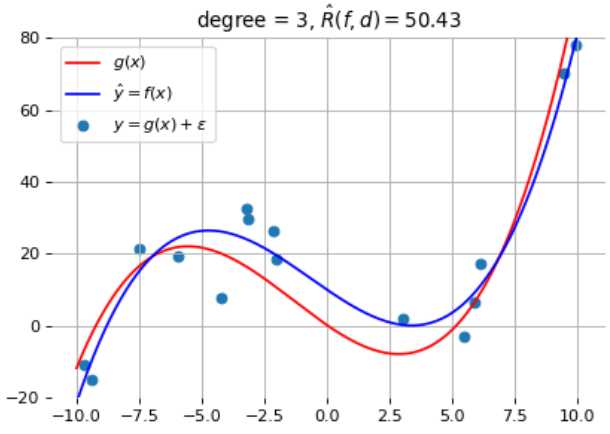
Case 2

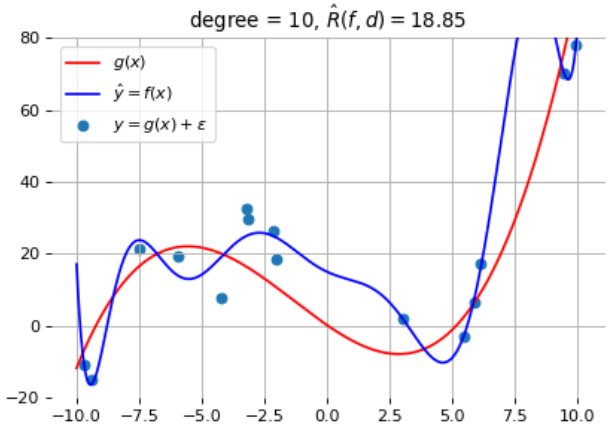
We have three different types of images to classify, cat, dog, and cow, where only cat images are noisy.



Case 3

What is the best model parameters that best explain a given dataset? What model structure should we use?





Case 1: Given a model trained with several pictures of dog breeds. We ask the model to decide on a dog breed using a photo of a cat.

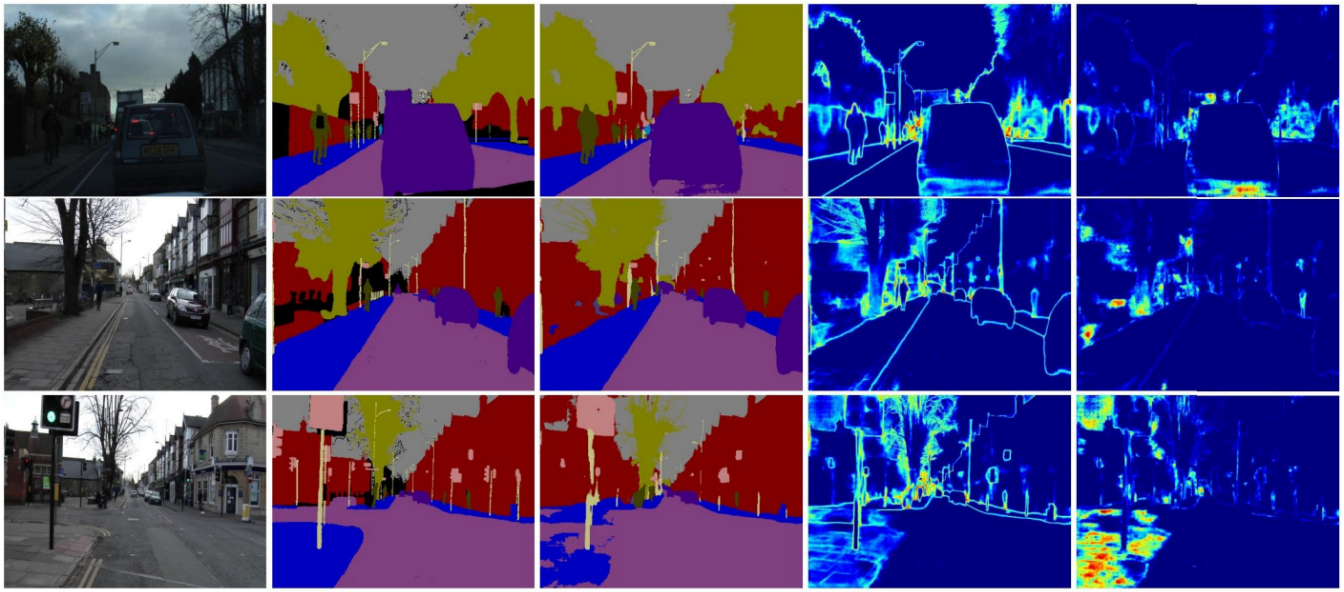
$\Rightarrow$ Out of distribution test data.

Case 2: We have three different types of images to classify, cat, dog, and cow, where only cat images are noisy.

$\Rightarrow$ Aleatoric uncertainty.

Case 3: What is the best model parameters that best explain a given dataset? What model structure should we use?

$\Rightarrow$ Epistemic uncertainty.



(a) Input Image (b) Ground Truth (c) Semantic Segmentation (d) Aleatoric Uncertainty (e) Epistemic Uncertainty

"Our model exhibits in (d) increased ***aleatoric uncertainty on object boundaries and for objects far from the camera****.* ***Epistemic uncertainty accounts for our ignorance about which model generated our collected data****. In (e) our model exhibits increased epistemic uncertainty for semantically and visually challenging pixels. The bottom row shows a failure case of the segmentation model when the model fails to segment the footpath due to increased epistemic uncertainty, but not aleatoric uncertainty."*

Credits: Kendall and Gal, What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision?, 2017.

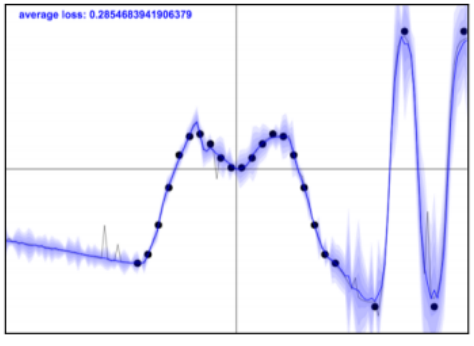
Aleatoric uncertainty

Aleatoric uncertainty captures noise inherent in the observations.

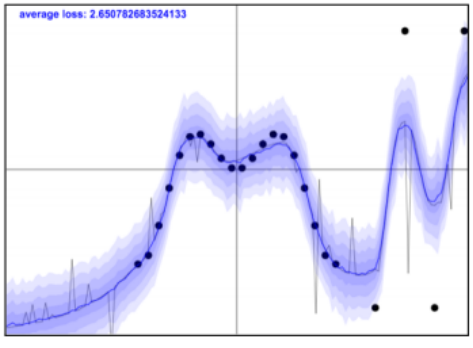
- For example, sensor noise or motion noise result in uncertainty.
- This uncertainty cannot be reduced with more data.
- However, aleatoric could be reduced with better measurements.

Aleatoric uncertainty can further be categorized into homoscedastic and heteroscedastic uncertainties:

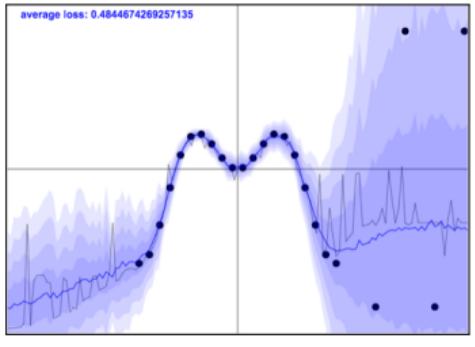
- Homoscedastic uncertainty relates to the uncertainty that a particular task might cause. It stays constant for different inputs.
- Heteroscedastic uncertainty depends on the inputs to the model, with some inputs potentially having more noisy outputs than others.



(a) Homoscedastic model with small observation noise.



(b) Homoscedastic model with large observation noise.



(c) Heteroscedastic model with data-dependent observation noise.

Credits: Yarin Gal, Uncertainty in Deep Learning, 2016.

Regression with uncertainty

Consider training data $(\mathbf{x}, y) \sim P(X, Y)$, with

- $\mathbf{x} \in \mathbb{R}^p$,
- $y \in \mathbb{R}$.

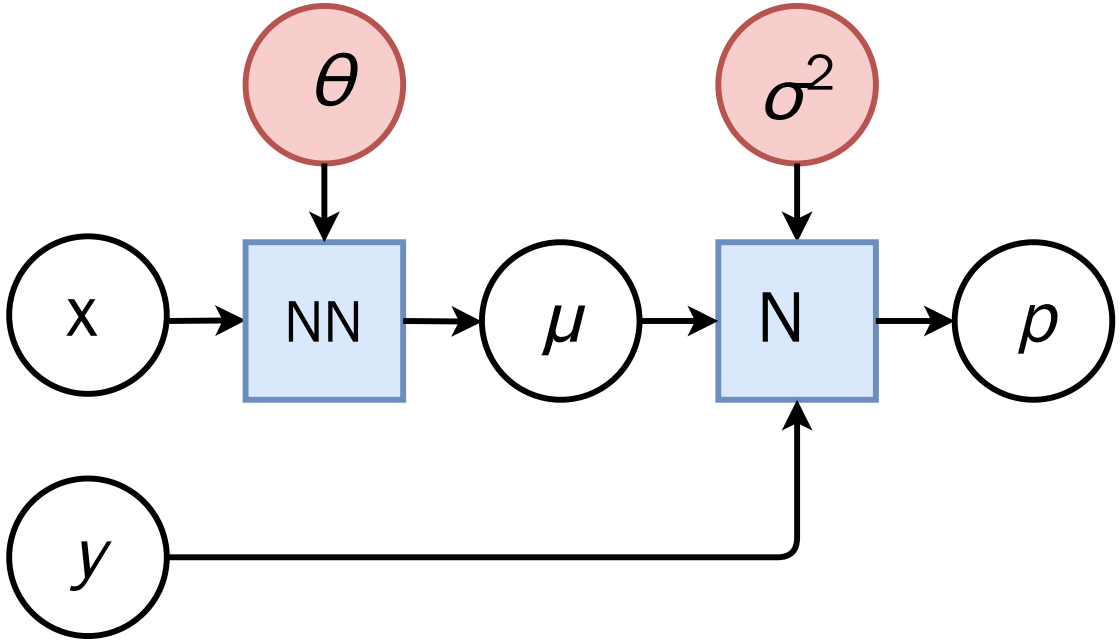
We model aleatoric uncertainty in the output by modelling the conditional distribution as a Normal distribution,

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

where $\mu(x)$ and $\sigma^2(\mathbf{x})$ are parametric functions to be learned, such as neural networks.

In particular, we do not wish to learn a function $\hat{y} = f(\mathbf{x})$ that would only produce point estimates.

Homoscedastic aleatoric uncertainty

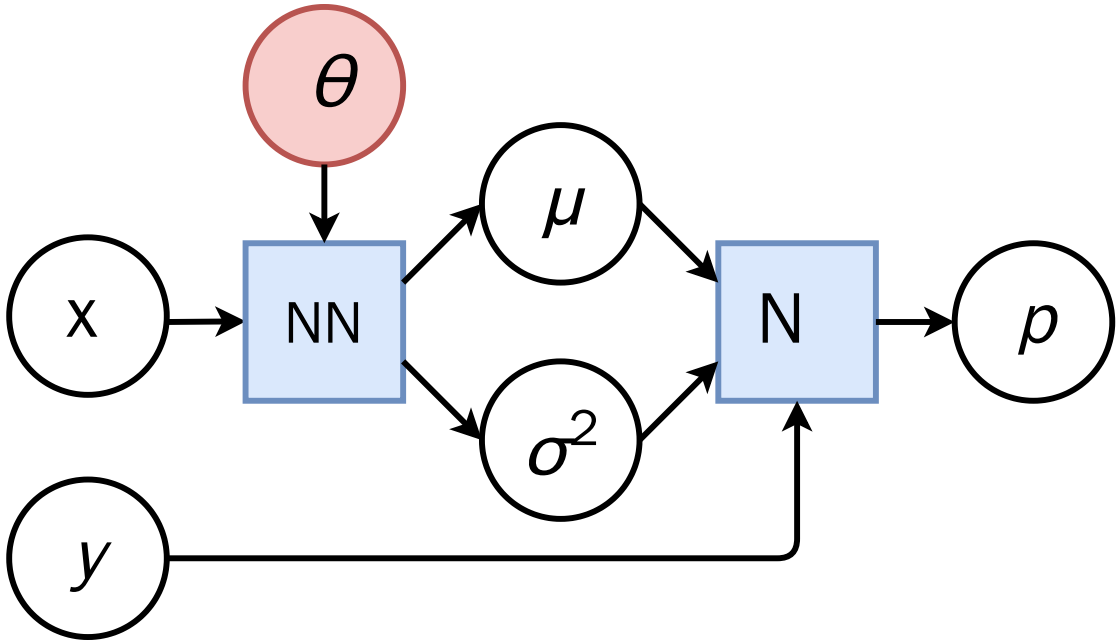


We have,

$$
\begin{aligned}
&\arg\max_{\theta,\sigma^2} p(\mathbf{d}|\theta,\sigma^2) \\
&= \arg\max_{\theta,\sigma^2} \prod_{\mathbf{x}_i,y_i\in\mathbf{d}} p(y_i|\mathbf{x}_i,\theta,\sigma^2) \\
&= \arg\max_{\theta,\sigma^2} \prod_{\mathbf{x}_i,y_i\in\mathbf{d}} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i-\mu(\mathbf{x}_i))^2}{2\sigma^2}\right) \\
&= \arg\min_{\theta,\sigma^2} \sum_{\mathbf{x}_i,y_i\in\mathbf{d}} \frac{(y_i-\mu(\mathbf{x}_i))^2}{2\sigma^2} + \log(\sigma) + C
\end{aligned}
$$

[Q] What if σ^2 was fixed?

Heteroscedastic aleatoric uncertainty



Same as for the homoscedastic case, except that that σ^2 is now a function of $\mathbf{x}_i$:

$$
\begin{aligned}
&\arg\max_{\theta} p(\mathbf{d}|\theta) \\
&= \arg\max_{\theta} \prod_{\mathbf{x}_i, y_i \in \mathbf{d}} p(y_i|\mathbf{x}_i, \theta) \\
&= \arg\max_{\theta} \prod_{\mathbf{x}_i, y_i \in \mathbf{d}} \frac{1}{\sqrt{2\pi}\sigma(\mathbf{x}_i)} \exp\left(-\frac{(y_i - \mu(\mathbf{x}_i))^2}{2\sigma^2(\mathbf{x}_i)}\right) \\
&= \arg\min_{\theta} \sum_{\mathbf{x}_i, y_i \in \mathbf{d}} \frac{(y_i - \mu(\mathbf{x}_i))^2}{2\sigma^2(\mathbf{x}_i)} + \log(\sigma(\mathbf{x}_i)) + C
\end{aligned}
$$

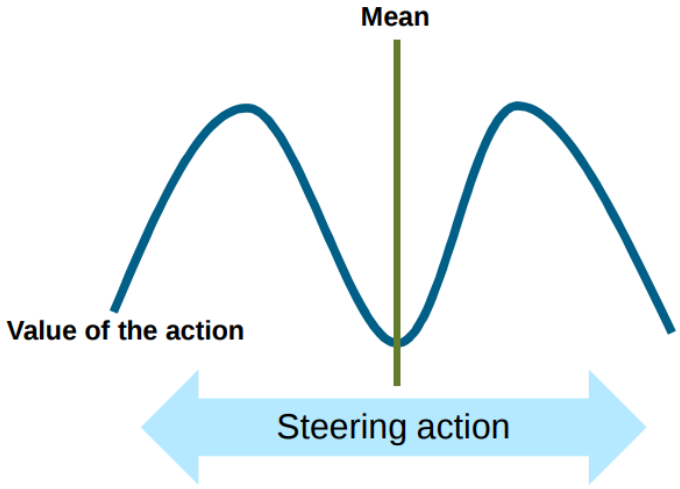
- What is the role of $2\sigma^2(\mathbf{x}_i)$?
- What about $\log(\sigma(\mathbf{x}_i))$?

Multimodality

Modelling $p(y|\mathbf{x})$ as a unimodal Gaussian is not always a good idea!

(and it would be even worse to have only point estimates for y!)

https://commons.wikimedia.org/wiki/File:Newport_Whitepit_Lane_pot_hole.JPG

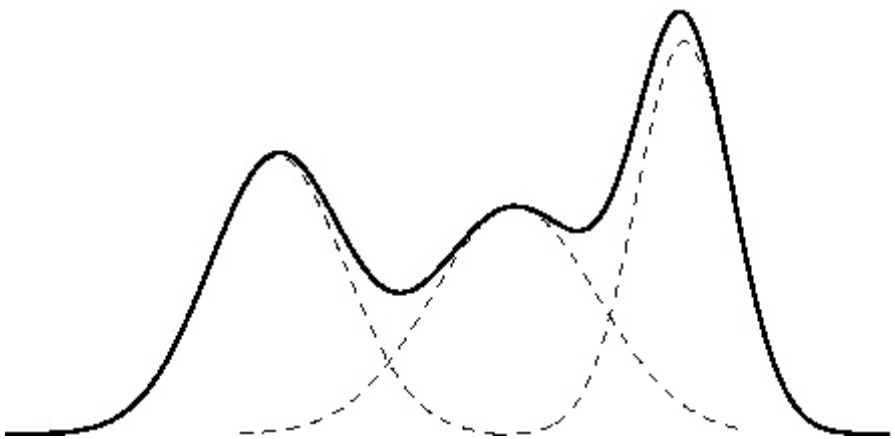


Gaussian mixture model

A Gaussian mixture model (GMM) defines instead $p(y|\mathbf{x})$ as a mixture of K Gaussian components,

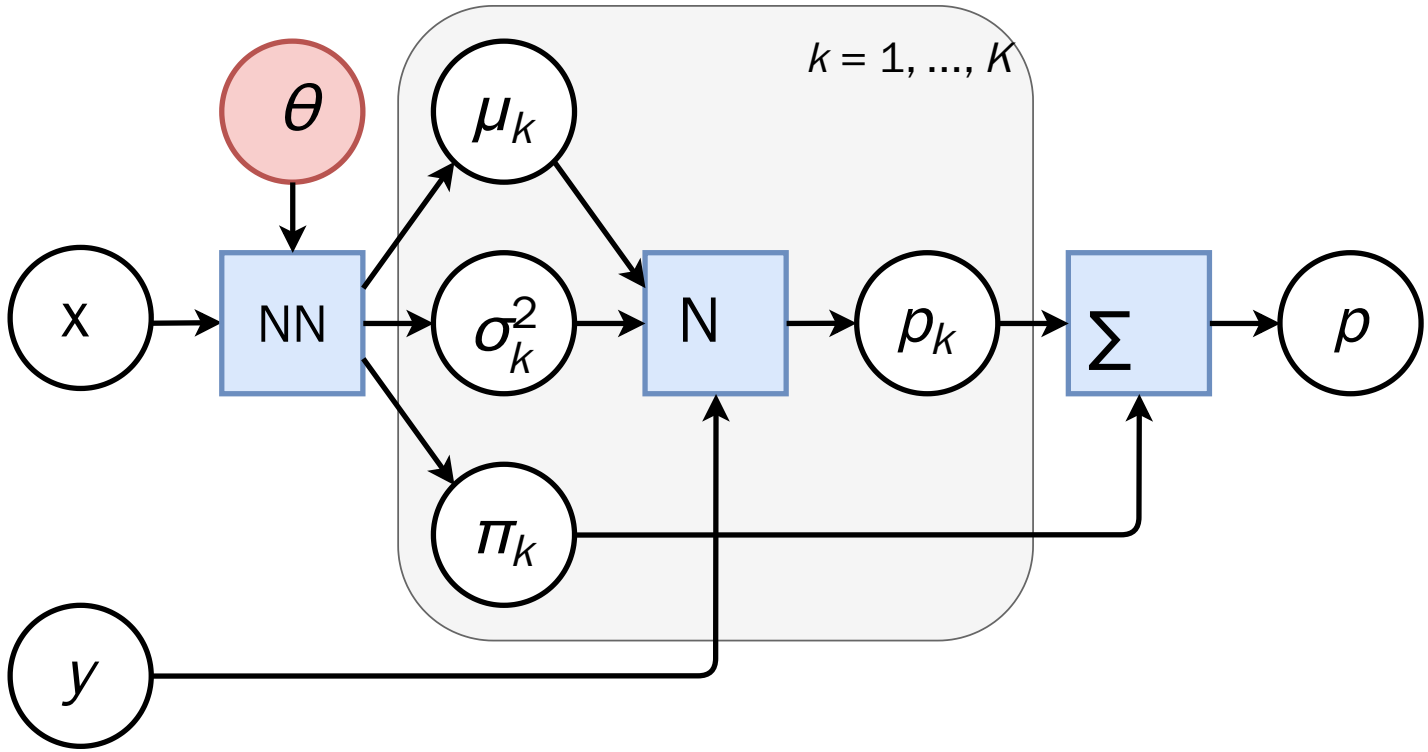
$$p(y|\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(y; \mu_k, \sigma_k^2),$$

where $0 \leq \pi_k \leq 1$ for all k and $\sum_{k=1}^{K} \pi_k = 1$.



Mixture density network

A mixture density network is a neural network implementation of the Gaussian mixture model.

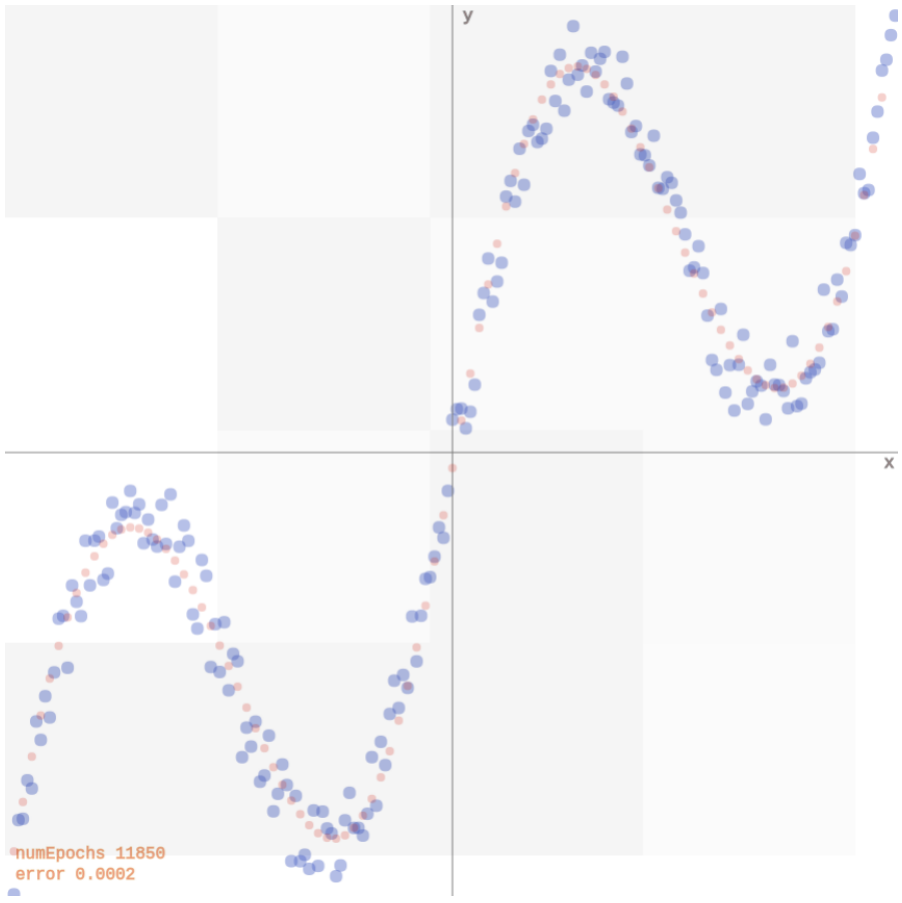


Illustration

Let us consider training data generated randomly as

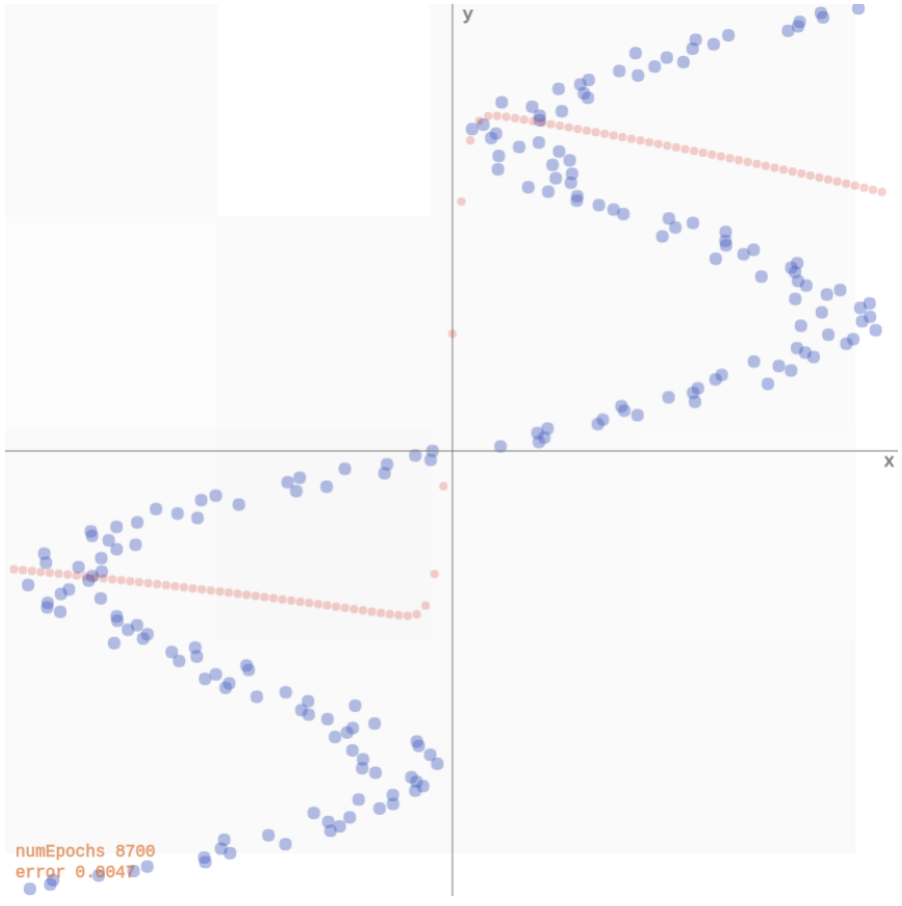
$$y_i = \mathbf{x}_i + 0.3 \sin(4\pi \mathbf{x}_i) + \epsilon_i$$

with $\epsilon_i \sim \mathcal{N}$.



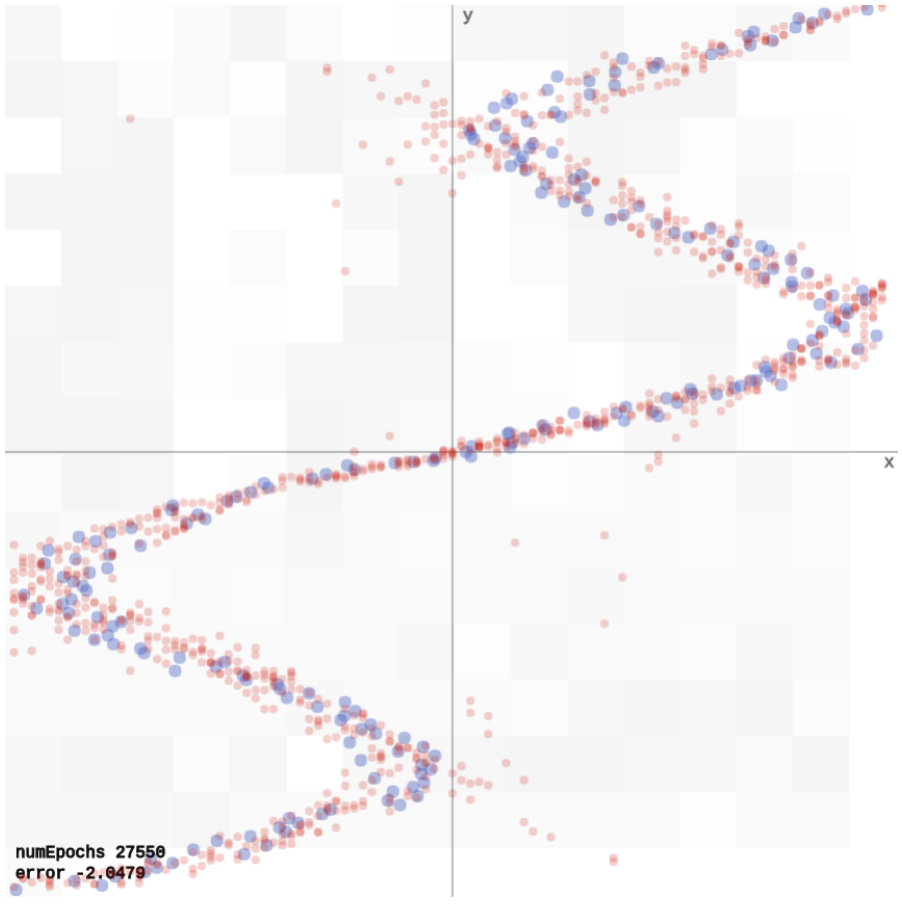
The data can be fit with a 2-layer network producing point estimates for y.
[demo]

Credits: David Ha, Mixture Density Networks, 2015.



If we flip $\mathbf{x}_i$ and y_i, the network faces issues since for each input, there are multiple outputs that can work. It produces some sort of average of the correct values. [demo]

Credits: David Ha, Mixture Density Networks, 2015.



A mixture density network models the data correctly, as it predicts for each input a distribution for the output, rather than a point estimate. [demo]

Credits: David Ha, Mixture Density Networks, 2015.

Epistemic uncertainty

Epistemic uncertainty accounts for uncertainty in the model parameters.

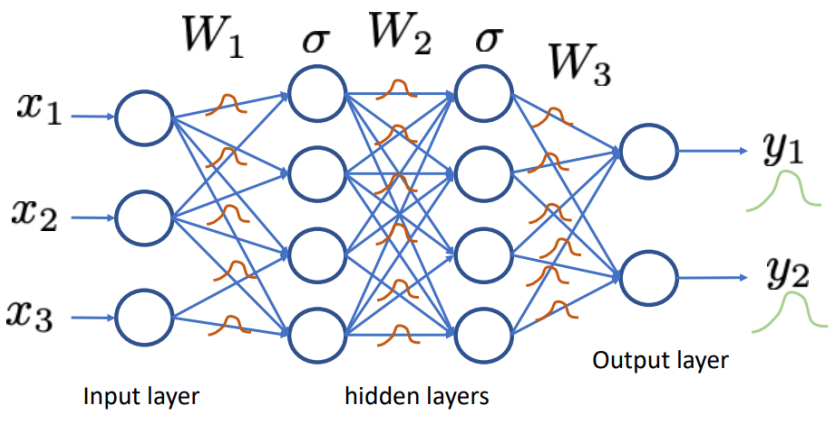
- It captures our ignorance about which model generated the collected data.
- It can be explained away given enough data (why?).
- It is also often referred to as model uncertainty.

Credits: Kendall and Gal, What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision?, 2017.

Bayesian neural networks

To capture epistemic uncertainty in a neural network, we model our ignorance with a prior distribution $p(\omega)$ over its weights.

Then we invoke Bayes for making predictions.



- The prior predictive distribution at $\mathbf{x}$ is given by integrating over all possible weight configurations,

$$p(y|\mathbf{x}) = \int p(y|\mathbf{x}, \omega) p(\omega) d\omega.$$

- Given training data $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ and $\mathbf{Y} = \{y_1, \ldots, y_N\}$, a Bayesian update results in the posterior

$$p(\omega|\mathbf{X}, \mathbf{Y}) = \frac{p(\mathbf{Y}|\mathbf{X}, \omega) p(\omega)}{p(\mathbf{Y}|\mathbf{X})}.$$

- The posterior predictive distribution is then given by

$$p(y|\mathbf{x}, \mathbf{X}, \mathbf{Y}) = \int p(y|\mathbf{x}, \omega) p(\omega|\mathbf{X}, \mathbf{Y}) d\omega.$$

Bayesian neural networks are easy to formulate, but notoriously difficult to perform inference in.

- This stems mainly from the fact that the marginal $p(\mathbf{Y}|\mathbf{X})$ is intractable to evaluate, which results in the posterior $p(\omega|\mathbf{X}, \mathbf{Y})$ not being tractable either.
- Therefore, we must rely on approximations.

Variational inference

Variational inference can be used for building an approximation $q(\omega; \nu)$ of the posterior $p(\omega|\mathbf{X}, \mathbf{Y})$.

As before (see Lecture 6), we can show that minimizing

$$\mathrm{KL}(q(\omega; \nu)||p(\omega|\mathbf{X}, \mathbf{Y}))$$

with respect to the variational parameters ν, is identical to maximizing the evidence lower bound objective (ELBO)

$$\mathrm{ELBO}(\nu) = \mathbb{E}_{q(\omega;\nu)} \left[\log p(\mathbf{Y}|\mathbf{X}, \omega)\right] - \mathrm{KL}(q(\omega; \nu)||p(\omega)).$$

The integral in the ELBO is not tractable for almost all q, but it can be minimized with stochastic gradient descent:

1. Sample $\hat{\omega} \sim q(\omega; \nu)$.
2. Do one step of maximization with respect to ν on

$$\hat{L}(\nu) = \log p(\mathbf{Y}|\mathbf{X}, \hat{\omega}) - \mathrm{KL}(q(\omega; \nu)||p(\omega))$$

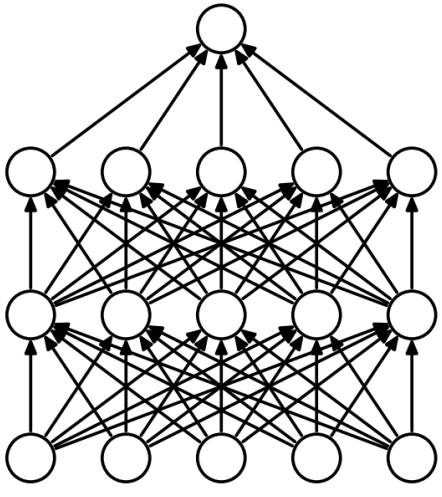
In the context of Bayesian neural networks, this procedure is also known as Bayes by backprop (Blundell et al, 2015).

Dropout

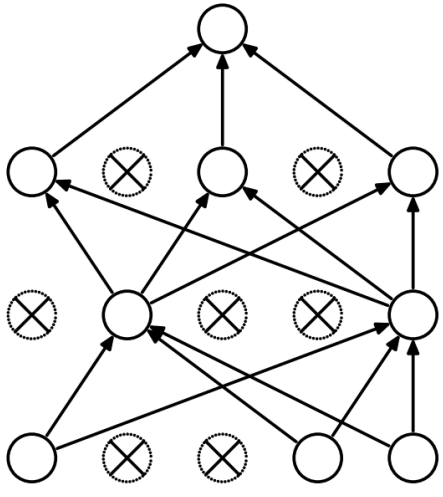
Dropout is an empirical technique that was first proposed to avoid overfitting in neural networks.

At each training step (i.e., for each sample within a mini-batch):

- Remove each node in the network with a probability p.
- Update the weights of the remaining nodes with backpropagation.



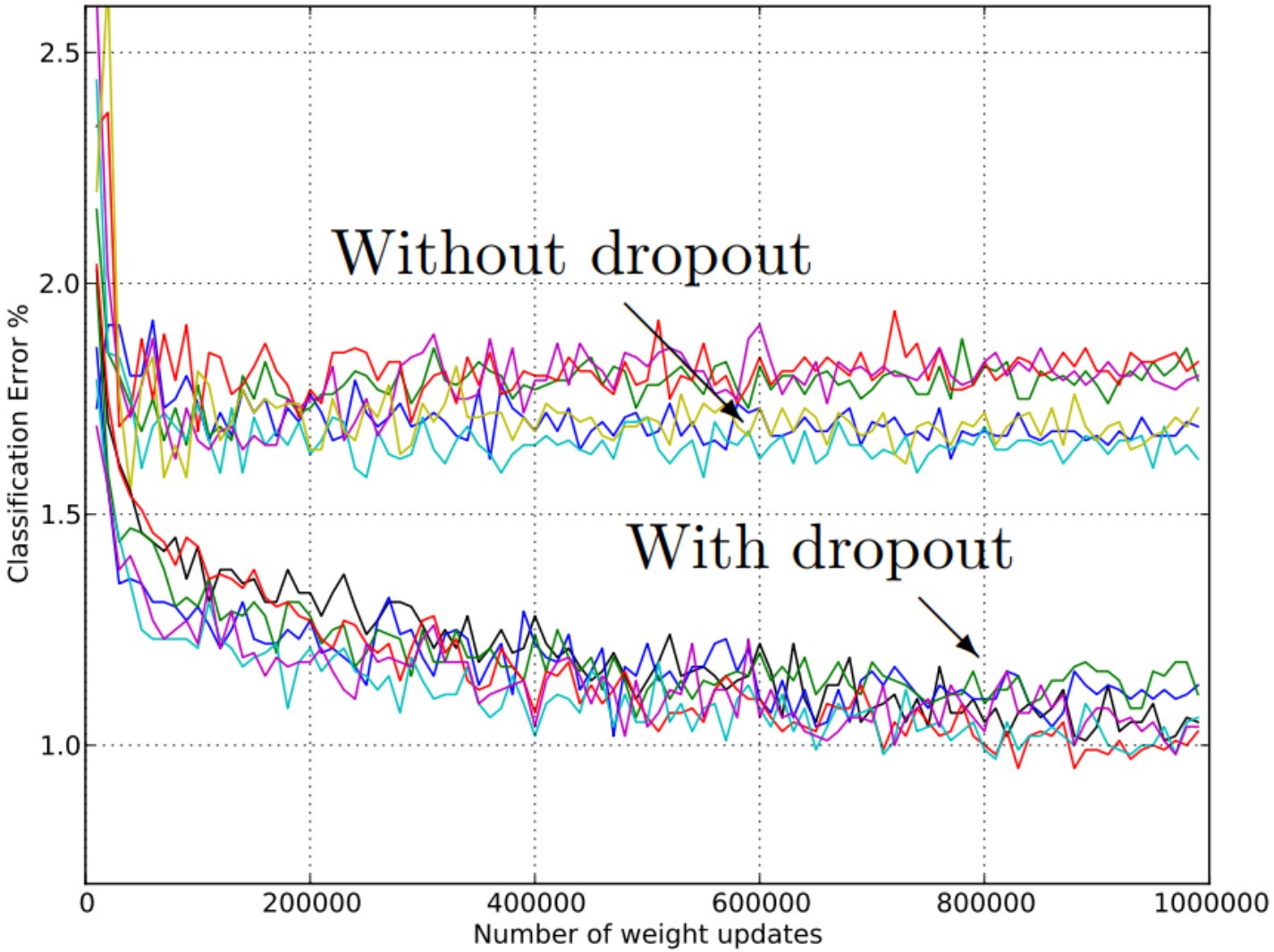
(a) Standard Neural Net



(b) After applying dropout.

At test time, either:

- Make predictions using the trained network without dropout but rescaling the weights by the dropout probability p (fast and standard).
- Sample T neural networks using dropout and average their predictions (slower but better principled).


Without dropout
With dropout
Classification Error %
2.5
2.0
1.5
1.0
0
200000
400000
600000
800000
1000000
Number of weight updates

Why does dropout work?

- It makes the learned weights of a node less sensitive to the weights of the other nodes.
- This forces the network to learn several independent representations of the patterns and thus decreases overfitting.
- It approximates Bayesian model averaging.

Dropout does variational inference

What variational family q would correspond to dropout?

- Let us split the weights ω per layer, $\omega = \{\mathbf{W}_1, ..., \mathbf{W}_L\}$, where $\mathbf{W}_i$ is further split per unit $\mathbf{W}_i = \{\mathbf{w}_{i,1}, ..., \mathbf{w}_{i,q_i}\}$.
- Variational parameters ν are split similarly into $\nu = \{\mathbf{M}_1, ..., \mathbf{M}_L\}$, with $\mathbf{M}_i = \{\mathbf{m}_{i,1}, ..., \mathbf{m}_{i,q_i}\}$.
- Then, the proposed $q(\omega; \nu)$ is defined as follows:

$$q(\omega; \nu) = \prod_{i=1}^{L} q(\mathbf{W}_i; \mathbf{M}_i)$$
$$q(\mathbf{W}_i; \mathbf{M}_i) = \prod_{k=1}^{q_i} q(\mathbf{w}_{i,k}; \mathbf{m}_{i,k})$$
$$q(\mathbf{w}_{i,k}; \mathbf{m}_{i,k}) = p\delta_0(\mathbf{w}_{i,k}) + (1-p)\delta_{\mathbf{m}_{i,k}}(\mathbf{w}_{i,k})$$

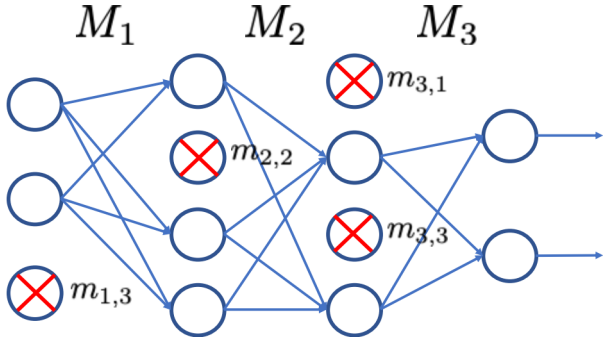
where $\delta_a(x)$ denotes a (multivariate) Dirac distribution centered at a.

Given the previous definition for q, sampling parameters $\hat{\omega} = \{\hat{\mathbf{W}}_1, ..., \hat{\mathbf{W}}_L\}$ is done as follows:

- Draw binary $z_{i,k} \sim \text{Bernoulli}(1-p)$ for each layer i and unit k.
- Compute $\hat{\mathbf{W}}_i = \mathbf{M}_i \text{diag}([z_{i,k}]_{k=1}^{q_i})$, where $\mathbf{M}_i$ denotes a matrix composed of the columns $\mathbf{m}_{i,k}$.

That is, $\hat{\mathbf{W}}_i$ are obtained by setting columns of $\mathbf{M}_i$ to zero with probability p.

This is strictly equivalent to dropout, i.e. removing units from the network with probability p.



Therefore, one step of stochastic gradient descent on the ELBO becomes:

1. Sample $\hat{\omega} \sim q(\omega; \nu) \Leftrightarrow$ Randomly set units of the network to zero $\Leftrightarrow$ Dropout.
2. Do one step of maximization with respect to $\nu = \{\mathbf{M}_i\}$ on

$$\hat{L}(\nu) = \log p(\mathbf{Y}|\mathbf{X}, \hat{\omega}) - \mathrm{KL}(q(\omega; \nu)||p(\omega)).$$

Maximizing $\hat{L}(\nu)$ is equivalent to minimizing

$$-\hat{L}(\nu) = -\log p(\mathbf{Y}|\mathbf{X}, \hat{\omega}) + \mathrm{KL}(q(\omega; \nu)||p(\omega))$$

Is this equivalent to one minimization step of a standard classification or regression objective? Yes!

- The first term is the typical objective (see Lecture 2).
- The second term forces q to remain close to the prior $p(\omega)$.
  - If $p(\omega)$ is Gaussian, minimizing the KL is equivalent to ℓ_2 regularization.
  - If $p(\omega)$ is Laplacian, minimizing the KL is equivalent to ℓ_1 regularization.

Conversely, this shows that when training a network with dropout with a standard classification or regression objective, one is actually implicitly doing variational inference to match the posterior distribution of the weights.

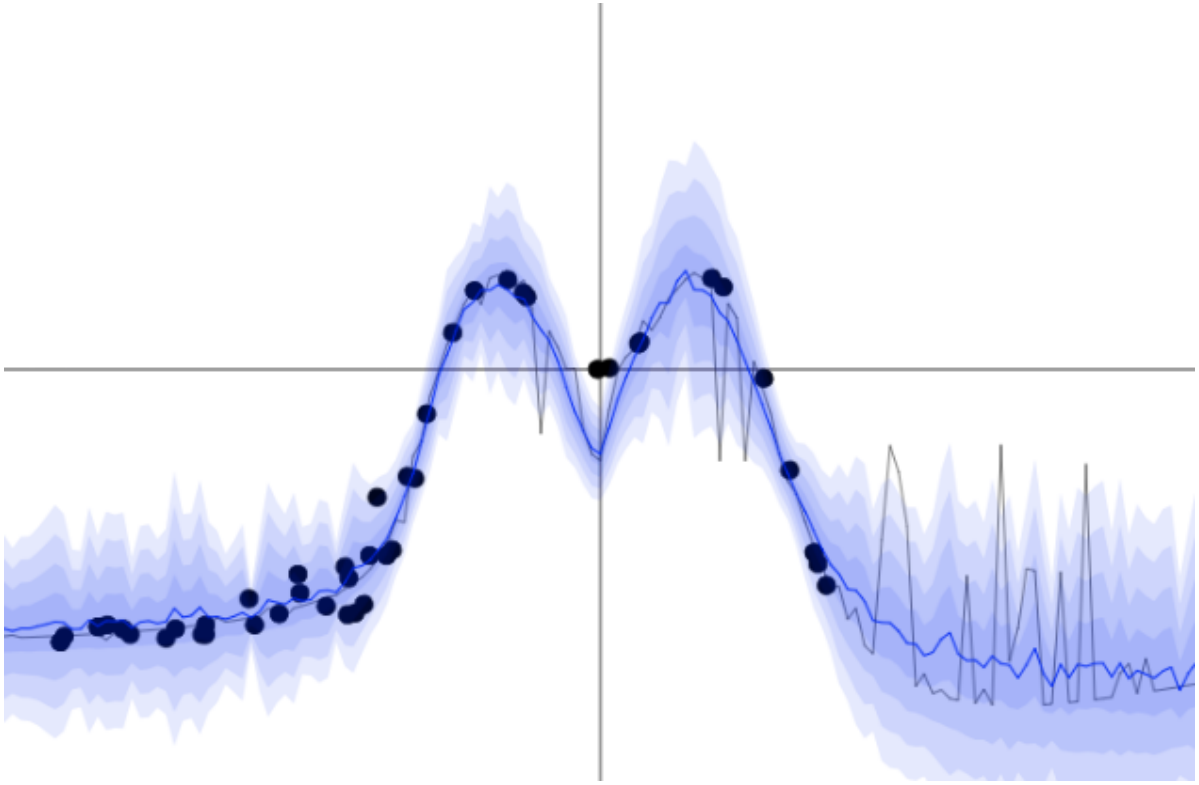
Uncertainty estimates from dropout

Proper epistemic uncertainty estimates at $\mathbf{x}$ can be obtained in a principled way using Monte-Carlo integration:

- Draw T sets of network parameters $\hat{\omega}_t$ from $q(\omega; \nu)$.
- Compute the predictions for the T networks, $\{f(\mathbf{x}; \hat{\omega}_t)\}_{t=1}^{T}$.
- Approximate the predictive mean and variance as follows:

$$\mathbb{E}_{p(y|\mathbf{x},\mathbf{X},\mathbf{Y})}[y] \approx \frac{1}{T}\sum_{t=1}^{T} f(\mathbf{x}; \hat{\omega}_t)$$

$$\mathbb{V}_{p(y|\mathbf{x},\mathbf{X},\mathbf{Y})}[y] \approx \sigma^2 + \frac{1}{T}\sum_{t=1}^{T} f(\mathbf{x}; \hat{\omega}_t)^2 - \hat{\mathbb{E}}[y]^2$$



Yarin Gal's demo.

Pixel-wise depth regression

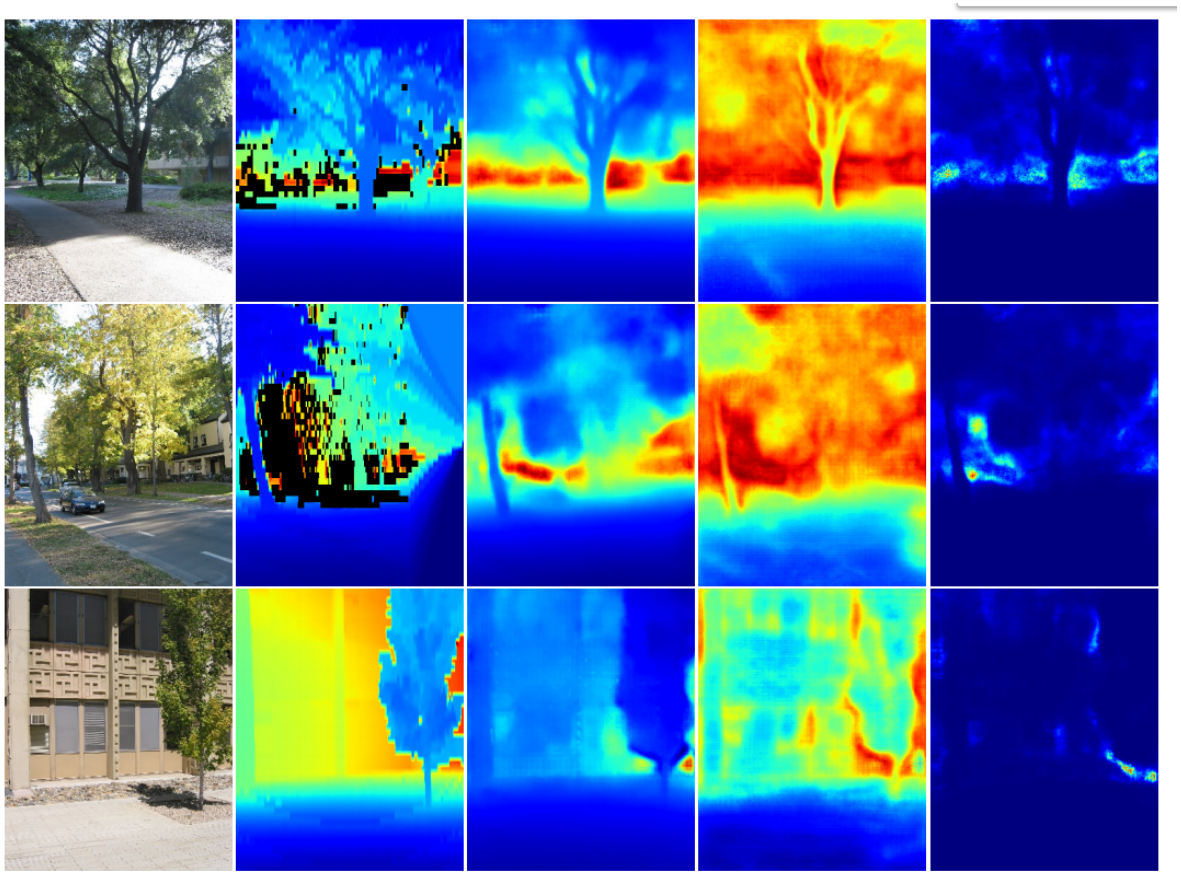


Figure 6: Qualitative results on the Make3D depth regression dataset. Left to right: input image, ground truth, depth prediction, aleatoric uncertainty, epistemic uncertainty. Make3D does not provide labels for depth greater than 70m, therefore these distances dominate the epistemic uncertainty signal. Aleatoric uncertainty is prevalent around depth edges or distant points.

Credits: Kendall and Gal, What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision?, 2017.

Bayesian Infinite Networks

Consider the 1-layer MLP with a hidden layer of size q and a bounded activation function σ:

$$f(x) = b + \sum_{j=1}^{q} v_j h_j(x)$$

$$h_j(x) = \sigma\left(a_j + \sum_{i=1}^{p} u_{i,j} x_i\right)$$

Assume Gaussian priors $v_j \sim \mathcal{N}(0, \sigma_v^2), b \sim \mathcal{N}(0, \sigma_b^2), u_{i,j} \sim \mathcal{N}(0, \sigma_u^2)$ and $a_j \sim \mathcal{N}(0, \sigma_a^2)$.

For a fixed value $x^{(1)}$, let us consider the prior distribution of $f(x^{(1)})$ implied by the prior distributions for the weights and biases.

We have

$$\mathbb{E}[v_j h_j(x^{(1)})] = \mathbb{E}[v_j]\mathbb{E}[h_j(x^{(1)})] = 0,$$

since v_j and $h_j(x^{(1)})$ are statistically independent and v_j has zero mean by hypothesis.

The variance of the contribution of each hidden unit h_j is

$$\begin{aligned}\mathbb{V}[v_j h_j(x^{(1)})] &= \mathbb{E}[(v_j h_j(x^{(1)}))^2] - \mathbb{E}[v_j h_j(x^{(1)})]^2 \\ &= \mathbb{E}[v_j^2]\mathbb{E}[h_j(x^{(1)})^2] \\ &= \sigma_v^2 \mathbb{E}[h_j(x^{(1)})^2],\end{aligned}$$

which must be finite since h_j is bounded by its activation function.

We define $V(x^{(1)}) = \mathbb{E}[h_j(x^{(1)})^2]$, and is the same for all j.

What if $q \to \infty$?

By the Central Limit Theorem, as $q \to \infty$, the total contribution of the hidden units, $\sum_{j=1}^{q} v_j h_j(x)$, to the value of $f(x^{(1)})$ becomes a Gaussian with variance $q\sigma_v^2 V(x^{(1)})$.

The bias b is also Gaussian, of variance σ_b^2, so for large q, the prior distribution $f(x^{(1)})$ is a Gaussian of variance $\sigma_b^2 + q\sigma_v^2 V(x^{(1)})$.

Accordingly, for $\sigma_v = \omega_v q^{-\frac{1}{2}}$, for some fixed ω_v, the prior $f(x^{(1)})$ converges to a Gaussian of mean zero and variance $\sigma_b^2 + \omega_v^2 \sigma_v^2 V(x^{(1)})$ as $q \to \infty$.

For two or more fixed values $x^{(1)}, x^{(2)}, \ldots$, a similar argument shows that, as $q \to \infty$, the joint distribution of the outputs converges to a multivariate Gaussian with means of zero and covariances of

$$\begin{aligned}\mathbb{E}[f(x^{(1)})f(x^{(2)})] &= \sigma_b^2 + \sum_{j=1}^{q} \sigma_v^2 \mathbb{E}[h_j(x^{(1)})h_j(x^{(2)})] \\ &= \sigma_b^2 + \omega_v^2 C(x^{(1)}, x^{(2)})\end{aligned}$$

where $C(x^{(1)}, x^{(2)}) = \mathbb{E}[h_j(x^{(1)})h_j(x^{(2)})]$ and is the same for all j.

This result states that for any set of fixed points $x^{(1)}, x^{(2)}, \ldots$, the joint distribution of $f(x^{(1)}), f(x^{(2)}), \ldots$ is a multivariate Gaussian.

In other words, the infinitely wide 1-layer MLP converges towards a Gaussian process.

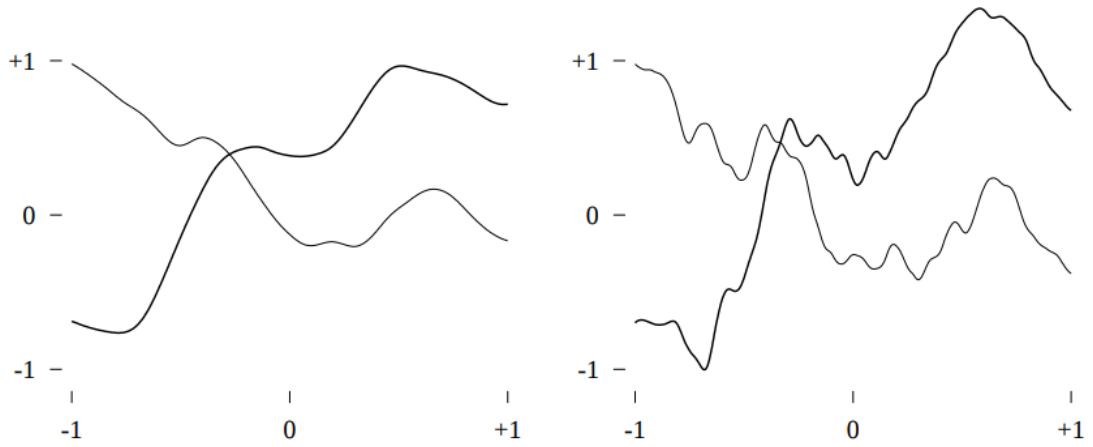


Figure 2.2: Functions drawn from Gaussian priors for a network with 10 000 tanh hidden units. Two functions drawn from a prior with $\sigma_u = 5$ are shown on the left, two from a prior with $\sigma_u = 20$ on the right. In both cases, $\sigma_a/\sigma_u = 1$ and $\sigma_b = \omega_v = 1$. The functions with different σ_u were generated using the same random number seed, the same as that used to generate the functions in the lower-right of Figure 2.1. This allows a direct evaluation of the effect of changing σ_u. (Use of a step function is equivalent to letting σ_u go to infinity, while keeping σ_a/σ_u fixed.)

(Neal, 1995)

The end.

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