Uncertainty Quantification - Bayesian Deep Models

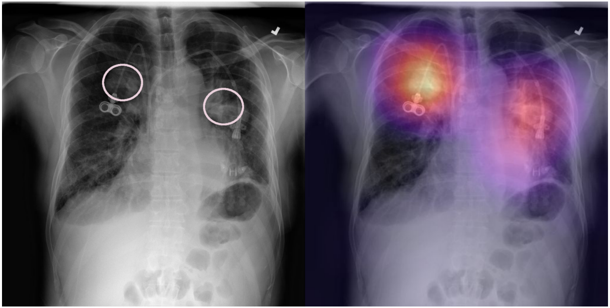
Clément Rambour

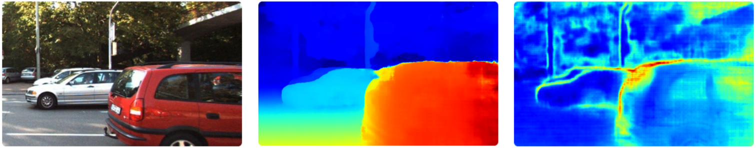
Sorbonne Université
ISIR - équipe MLIA

Robustness in Deep Learning

Deep Learning : huge gain in average performance, *e.g.* precision for classification

- Need for **performance certification in safety-critical applications : robustness**
  - Healthcare, autonomous steering, nuclear, defense, *etc*

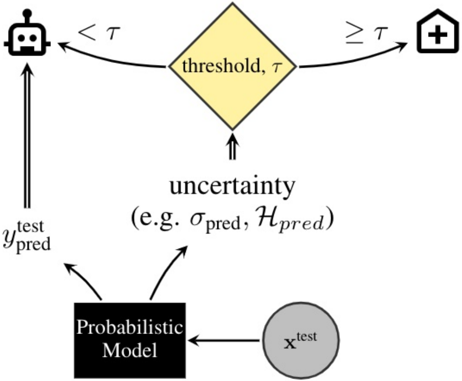




Robustness in Deep Learning

Performance certification

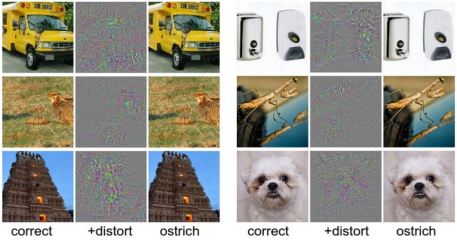
- **Reliable confidence / uncertainly estimation** of the decision process
  - "Know when you do not know"



Robustness in Deep Learning

Performance certification

- <u>**Stability of the decision function**</u>, *e.g.* robustness to adversarial attacks



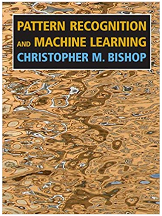
[Evtimov et al., 2017]

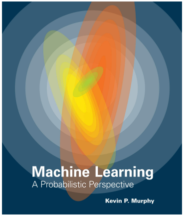
Robustness in Deep Learning : RDFIA Section 4

2 seances on robust deep learning

1. **Week 1 :** Bayesian models and uncertainty estimation
2. **Week 2 :** Application of uncertainty : failure prediction, OOD detection

- **References :**
  - Pattern Recognition and Machine Learning [Bishop, 2006]
  - Machine Learning : A Probabilistic Perspective [Murphy, 2012]





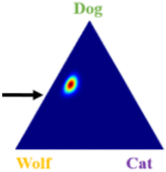
Outline

Type of uncertainties

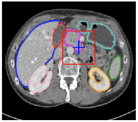
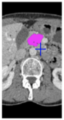
Aleatoric uncertainty

- *Aleator* (lat.) = dice player
- **Noise inherent in the observations**, *i.e.* natural randomness.
  - Inherent stochasticity, *e.g.* class confusion



  - Ambiguous data (*e.g.* medical images), or sensor quality

*Rain drops**


Lack of visual features


Glare

Type of uncertainties

Aleatoric uncertainty

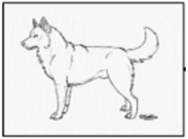
- *aleator* (lat.) = dice player
- **Noise inherent in the observations**, *i.e.* natural randomness.
- Cannot be reduced (need to change input/sensor), but can be estimated/learned
- Two (sub)-types of aleatoric uncertainty :
  1. **homoscedastic uncertainty** : stays constant for different input values, limited, captures 'average' uncertainty
  2. **heteroscedastic uncertainty** : depends on the input, learned from data

Type of uncertainties

Epistemic uncertainty

- *Episteme* (gr.) : knowledge $\Rightarrow$ **model uncertainty**
- Lack of knowledge about the generating process y (class) $\rightarrow$ input (image)



- **Main feature :** detects samples far from the training distribution
- Can be explained away given enough data
  - Epistemic uncertainty $\downarrow$ when number of data N (evidence) $\uparrow$
  - Epistemic uncertainty $\rightarrow 0$ when $N \rightarrow \infty$

Outline

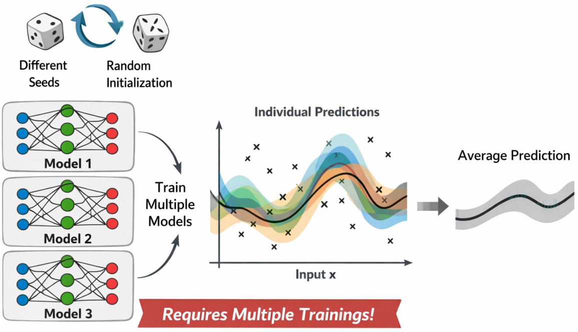
Uncertainty quantification

Intuition

How to assess the stability of a given model with respect to a training set ?

Naively :

- train multiple models with varying seed / initialization
- Average predictions on the input space to obtain an empirical distribution over the model outputs
  $\hookrightarrow$ Requires multiple training



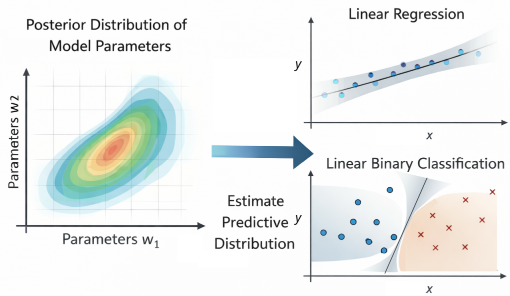
Bayesian Models

Intuition

How to assess the stability of a given model with respect to a training set ?

Bayesian approach :

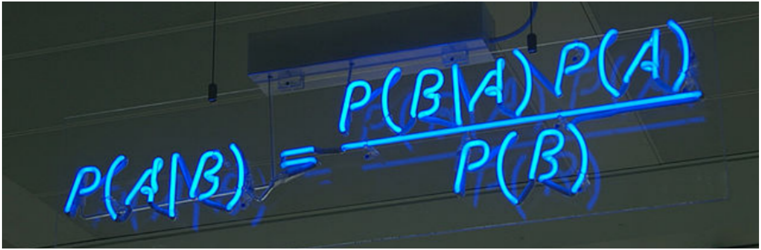
- Estimate the model distribution ⇔ the distribution of the model's parameters
- Estimate the predictive ditribution ⇔ distribution of the prediction in the input space



Bayesian Models

- Dataset $\mathcal{D} = (\mathbf{X}, \mathbf{Y})$ with inputs $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^N$ and outputs $\mathbf{Y} = \{\mathbf{y}_i\}_{i=1}^N$
  - $\mathbf{x}_i \in \mathbb{R}^d$, $\mathbf{y}_i^* \in \mathbb{R}^K$ (classification or regression)
  - Model with parameters $\mathbf{w}$: $\hat{\mathbf{y}}_i = f_{\mathbf{w}}(\mathbf{x}_i)$
- **Bayes rule :** $p(\mathbf{Y}, \mathbf{w}/\mathbf{X}) = p(\mathbf{Y}/\mathbf{X}, \mathbf{w})p(\mathbf{w}) = p(\mathbf{w}/\mathbf{X}, \mathbf{Y})p(\mathbf{Y}/\mathbf{X})$

$$\Rightarrow \boxed{p(\mathbf{w}/\mathbf{X}, \mathbf{Y}) = \frac{p(\mathbf{Y}/\mathbf{X},\mathbf{w})p(\mathbf{w})}{p(\mathbf{Y}/\mathbf{X})} \propto p(\mathbf{Y}/\mathbf{X}, \mathbf{w})p(\mathbf{w})}$$



Bayesian Models

Deterministic *vs.* Bayesian learning

- **Deterministic models** learn the model's parameters $\mathbf{w}$ on the training set $\mathcal{D}$ that minimizes the expected loss $\mathcal{L}$:

$$\mathbf{w} = \underbrace{\operatorname{argmin}_{\mathbf{w}}}_{\substack{\text{find best} \\ \text{fixed parameters}}} \quad \underbrace{\mathbb{E}_{(\mathbf{x},\mathbf{y})\sim p(\mathcal{D})}}_{\substack{\text{data sampled} \\ \text{from } \mathcal{D}}} \quad \mathcal{L}\big(f_{\mathbf{w}}(\mathbf{x}), \mathbf{y}\big)$$

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- **Bayesian models** learn the distribution of $\mathbf{w}$ given the training set $p(\mathbf{w}|\mathcal{D})$. The best model $\mathbf{w}^*$ is called the maximum a posteriori (MAP) :

$$\mathbf{w}^* = \underbrace{\operatorname*{argmin}_{\mathbf{w}}}_{\substack{\text{find best parameters}\\ \text{from their distribution}}} -\log \underbrace{p(\mathbf{w}|\mathcal{D})}_{\substack{\text{parameters conditional}\\ \text{distribution}}}$$

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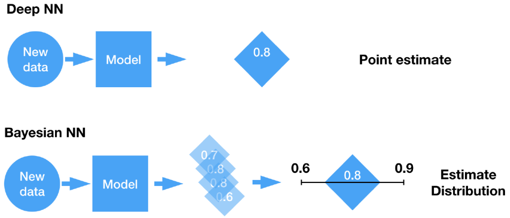


Bayesian Models & Uncertainty

Predictive distribution

From posterior $p(\mathbf{w}|\mathcal{D})$ $\Rightarrow$ compute **predictive distribution** given new input $\mathbf{x}^*$:

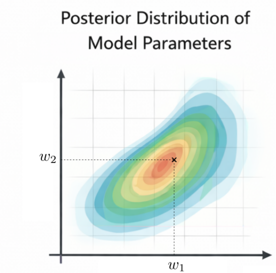
$$\forall y, \quad p(\mathbf{y}|\mathbf{x}^*, \mathcal{D}) = \int \boxed{p(\mathbf{y}, \mathbf{w}|\mathbf{x}^*, \mathcal{D})} d\mathbf{w} \quad \text{marginalization}$$

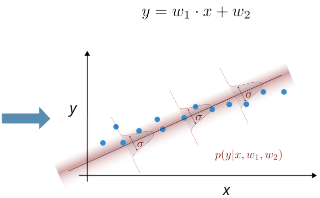
Bayes

$$= \int \boxed{p(\mathbf{y}|\mathbf{x}^*, \mathbf{w})} \; \boxed{p(\mathbf{w}|\mathcal{D})} d\mathbf{w} \quad \text{Bayes rule}$$

$$= \mathbb{E}_{p(\mathbf{w}|\mathcal{D})}[p(y|\mathbf{x}^*, \mathbf{w})] \quad \text{expectation definition}$$

Naturally gives a measure of uncertainty





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$$
\begin{aligned}
\forall y, \quad p(\mathbf{y}|\mathbf{x}^*, \mathcal{D}) &= \int \boxed{p(\mathbf{y}, \mathbf{w}|\mathbf{x}^*, \mathcal{D})} d\mathbf{w} && \text{marginalization} \\
& \qquad \text{Bayes} \\
&= \int \boxed{p(\mathbf{y}|\mathbf{x}^*, \mathbf{w})} \; \boxed{p(\mathbf{w}|\mathcal{D})} d\mathbf{w} && \text{Bayes rule} \\
&= \mathbb{E}_{p(\mathbf{w}|\mathcal{D})}\left[p(y|\mathbf{x}^*, \mathbf{w})\right] && \text{expectation definition}
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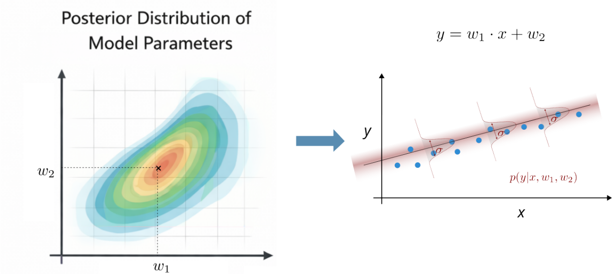
Naturally gives a measure of uncertainty



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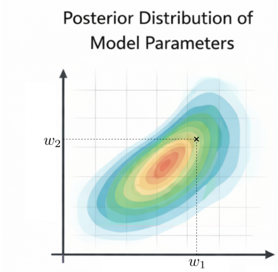

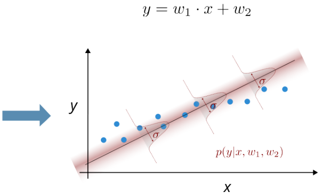

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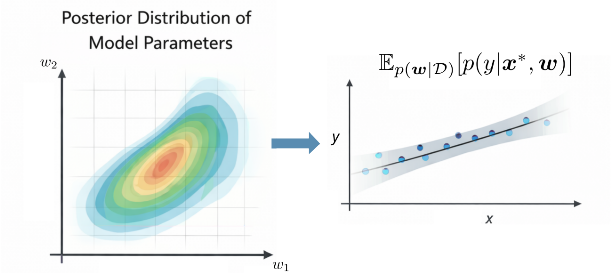
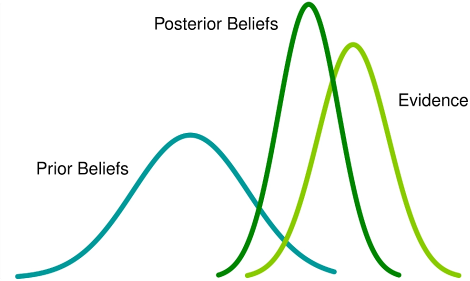


Bayesian Models & Uncertainty

- RECAP : for uncertainty estimate with Bayesian models
  1. Define prior $p(\mathbf{w})$ and likelihood $p(\mathbf{Y}/\mathbf{X}, \mathbf{w})$
  2. Compute posterior distribution $p(\mathbf{w}/\mathbf{X}, \mathbf{Y})$
  3. Compute predictive distribution $p(\mathbf{y}^*/\mathbf{x}^*, \mathbf{Y}, \mathbf{X})$
- Easy ? NO ! ! $\Rightarrow$ steps 2 and 3 computationally hard in general !
  - Typically no closed form for step 2
  - High-dimensional integration for step 3



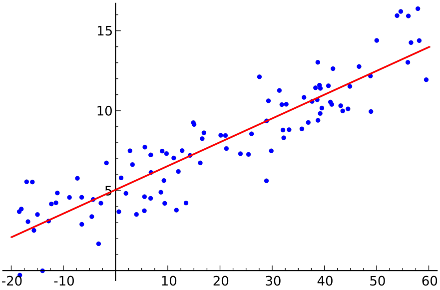
Probabilistic Linear Regression

- N training examples $(\mathbf{x}_i, \mathbf{y}_i)_{i \in \{1;N\}}$; $\mathbf{x}_i \in \mathbb{R}^p$, $\mathbf{y}_i \in \mathbb{R}^K$
- Matrix notation including bias in $\mathbf{w}$: $\mathbf{\Phi}$ of size $N \times (p+1)$

$$\mathbf{\Phi} = \begin{pmatrix} 1 & x_{11} & \dots & x_{1p} \\ 1 & x_{21} & \dots & x_{2p} \\ \dots & \dots & \dots & \dots \\ 1 & x_{N1} & \dots & x_{Np} \end{pmatrix}$$

- $\boxed{\mathbf{Y} = \mathbf{\Phi}\mathbf{w} + \boldsymbol{\varepsilon}}$, $\boldsymbol{\varepsilon} \in \mathbb{R}^{N \times K}$, $\varepsilon_{i,k} \sim \mathcal{N}(0, \sigma^2)$
- $\mathbf{Y} \in \mathbb{R}^{N \times K}$, $\mathbf{\Phi} \in \mathbb{R}^{N \times (p+1)}$, $\mathbf{w} \in \mathbb{R}^{(p+1) \times K}$
  - $\mathbf{\Phi}_i^T := \begin{pmatrix} 1 & x_{i1} & \dots & x_{ip} \end{pmatrix}^T \in \mathbb{R}^{1 \times (p+1)}$
  - $\mathbf{y}_i = \mathbf{\Phi}_i^T \mathbf{w} + \varepsilon_i$, $\mathbf{y}_i \in \mathbb{R}^{1 \times K}$, $\varepsilon_i \in \mathbb{R}^{1 \times K}$

- Ex : scalar inputs and outputs $p = 1$, $K = 1 \Rightarrow \mathbf{\Phi} \in \mathbb{R}^{N \times 2}$, $\mathbf{w} \in \mathbb{R}^2$:



Probabilistic Linear Regression

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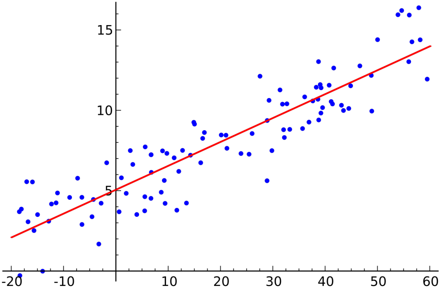
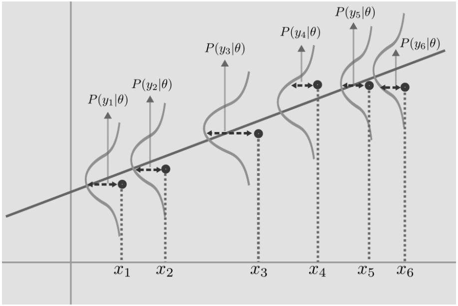
- $p(\mathbf{y}_i / \mathbf{x}_i, \mathbf{w}) \sim \mathcal{N}(\mathbf{\Phi}_i^T \mathbf{w}, \sigma^2)$ or $p(\mathbf{y}_i - \mathbf{\Phi}_i^T \mathbf{w}) \sim \mathcal{N}(0, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma}\, e^{\frac{(\mathbf{y}_i - \mathbf{\Phi}_i^T \mathbf{w})^2}{2\sigma^2}}$
  - $p(\mathbf{y}_i / \mathbf{x}_i, \mathbf{w})$: likelihhod, $\sigma \sim$ aleatoric uncertainty
  - σ independent of $\mathbf{x} \Rightarrow$ homoscedastic uncertainty





Probabilistic Linear Regression

- Trained with Maximum Likelihood (ML)
  - Examples assumed to be *i.i.d* (independent and identically distributed)
    $\Rightarrow p(\mathbf{Y}/\mathbf{X}, \mathbf{w}, \sigma) = \prod_{i=1}^{N} p(y_i/x_i, \mathbf{w}, \sigma)$
  - MLE : $(\hat{\mathbf{w}}, \hat{\sigma}) = \arg\max_{(\mathbf{w},\sigma)} p(\mathbf{X}, \mathbf{Y}/\mathbf{w}, \sigma) = \arg\min_{\mathbf{w},\sigma} - \sum_{i=1}^{N} log\left[p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w})\right]$

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- MLE solution $\mathbf{w}$: $\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} C(\mathbf{w}) = \arg\min_{\mathbf{w}} \sum_{i=1}^{N} (\mathbf{y}_i - \mathbf{\Phi}_i^T \mathbf{w})^2$

  $\Rightarrow$ Ordinary least square problem (closed form) :
  - $C(\mathbf{w}) = ||\mathbf{Y} - \mathbf{\Phi w})||^2 = (\mathbf{Y} - \mathbf{\Phi w})^T(\mathbf{Y} - \mathbf{\Phi w}),\ \nabla_{\mathbf{w}} C = 2\mathbf{\Phi}^T(Y - \mathbf{\Phi w})$
  - $\nabla_{\mathbf{w}} C = 0 \Leftrightarrow \mathbf{\Phi}^T\mathbf{\Phi w}^{=}\mathbf{\Phi}^T\mathbf{Y}$

$$\boxed{\hat{\mathbf{w}} = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{Y}}$$

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- ML solution σ : $\arg\min_{\sigma}[\ N\ log(\sigma) + \frac{1}{2\sigma^2} \sum_{i=1}^{N} (\mathbf{y}_i - \mathbf{\Phi}_i^T \mathbf{w})^2]$
  - Closed form solution : $\hat{\sigma^2} = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{y}_i - \mathbf{\Phi}_i^T \mathbf{w})^2 \Rightarrow$ interpretation : data std

Limits of MLE

- Learning model to predict coin toss with MLE
  - Bernoulli variable $\mathbf{X}$ with param p : $P(\mathbf{x}|p) = \prod_{i=1}^{N} P(x_i|p) = \prod_{i=1}^{N} p^{x_i}(1-p)^{1-x_i}$
  - MLE : $\ln P(\mathbf{x}|p) = \sum_{i=1}^{N} [x_i \ln p + (1-x_i)\ln(1-p)] \Rightarrow \boxed{p_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i}$
  - MLE : predict $P(X|p_{MLE}) = 1$ for all futures tosses !

- Using prior knowledge on p, *e.g.* $P(p) = 0.5$ or $P(p) = 0.3 \Rightarrow$ MAP

Bayesian Linear Regression

$$\boxed{\text{Include prior } p(\mathbf{w}) \Rightarrow \text{biased posterior } p(\mathbf{w}/\mathbf{X},\mathbf{Y}) \text{ (MAP)}}$$

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- Choose **Prior**, *e.g.* $p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}; 0, \alpha^{-1}I)$

Bayesian Linear Regression

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- **Likelihood**, as before : $p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w}) = \mathcal{N}(\mathbf{\Phi}_i^T \mathbf{w}, \beta^{-1})$ with $\beta = \frac{1}{2\sigma^2}$
  $\Rightarrow$ **Compute posterior** $p(\mathbf{w}/\mathbf{x}_i, \mathbf{y}_i) \propto p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w})p(\mathbf{w})$

Bayesian Linear Regression

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- Choose **Prior**, *e.g.* $p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}; 0, \alpha^{-1}I)$
- **Likelihood**, as before : $p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w}) = \mathcal{N}(\mathbf{\Phi}_i^T\mathbf{w}, \beta^{-1})$ with $\beta = \frac{1}{2\sigma^2}$
  $\Rightarrow$ **Compute posterior** $p(\mathbf{w}/\mathbf{x}_i, \mathbf{y}_i) \propto p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w})p(\mathbf{w})$
  - Here, prior same form as likelihood (Gaussian), *i.e.* **Prior conjugate to likelihood**
    $\Rightarrow$ **Posterior as the same form as the prior**
    $\Rightarrow$ **Closed-form for the posterior, which is also Gaussian !**

Bayesian Linear Regression

$$\boxed{\text{Include prior } p(\mathbf{w}) \Rightarrow \text{biased posterior } p(\mathbf{w}/\mathbf{X},\mathbf{Y}) \text{ (MAP)}}$$

- Choose **Prior**, *e.g.* $p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}; 0, \alpha^{-1}I)$
- **Likelihood**, as before : $p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w}) = \mathcal{N}(\mathbf{\Phi}_i^T\mathbf{w}, \beta^{-1})$ with $\beta = \frac{1}{2\sigma^2}$
  $\Rightarrow$ **Compute posterior** $p(\mathbf{w}/\mathbf{x}_i, \mathbf{y}_i) \propto p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w})p(\mathbf{w})$
  - Here, prior same form as likelihood (Gaussian), *i.e.* **Prior conjugate to likelihood**
    $\Rightarrow$ **Posterior as the same form as the prior**
    $\Rightarrow$ **Closed-form for the posterior, which is also Gaussian !**
  - With $p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}; 0, \alpha^{-1}I)$ and $p(\mathbf{y}_i/\mathbf{x}_i, \mathbf{w}) = \mathcal{N}(\mathbf{\Phi}_i^T\mathbf{w}, \beta^{-1})$, we can show that :

$$\boxed{\begin{aligned} p(\mathbf{w}/\mathbf{X},\mathbf{Y}) &= \mathcal{N}(\mathbf{w}|\boldsymbol{\mu}, \mathbf{\Sigma}) \\ \mathbf{\Sigma}^{-1} &= \alpha \boldsymbol{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi} \\ \boldsymbol{\mu} &= \beta \mathbf{\Sigma} \mathbf{\Phi}^T \mathbf{Y} \end{aligned}}$$

- Closed form solution for MAP ($\boldsymbol{\mu}$, median $\leftrightarrow$ mode)
- $\alpha \to 0 \Rightarrow$ recover ML ; $N = 0 \Rightarrow$ recover prior

Bayesian Linear Regression

Come from general results [Bishop, 2006]

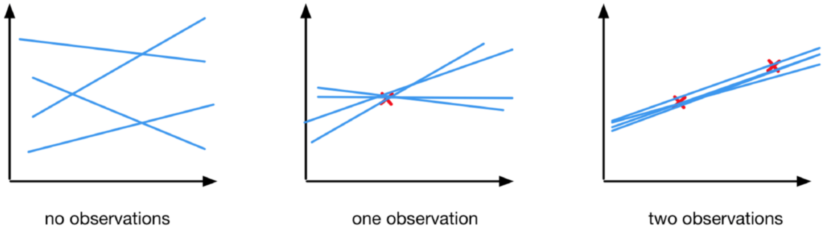
- Assume that :
  - $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_x)$
  - $p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}|A\mathbf{x} + b, \boldsymbol{\Sigma}_y)$
- Then : $p(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{x|\mathbf{y}}, \boldsymbol{\Sigma}_{x|\mathbf{y}})$, with :

$$\boldsymbol{\Sigma}_{\boldsymbol{x}|\mathbf{y}}^{-1} = \boldsymbol{\Sigma}_x^{-1} + \boldsymbol{A}^T \boldsymbol{\Sigma}_y^{-1} \boldsymbol{A}$$

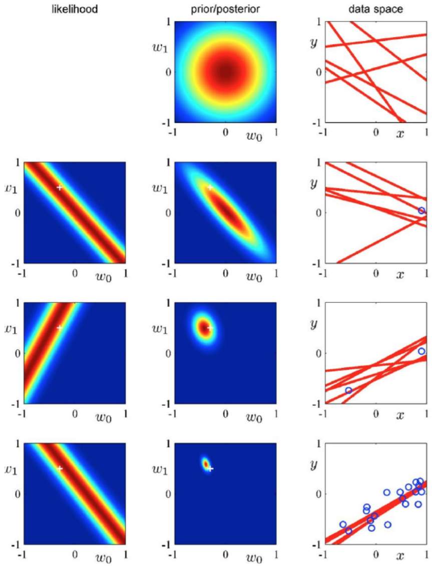
$$\boldsymbol{\mu}_{x|\mathbf{y}} = \boldsymbol{\Sigma}_{\boldsymbol{x}|\mathbf{y}}[A^T \boldsymbol{\Sigma}_y^{-1}(\mathbf{y} - b) + \boldsymbol{\Sigma}_x^{-1} \boldsymbol{\mu}_x]$$

Bayesian Linear Regression : Posterior Sampling

- $p(\mathbf{w}/\mathbf{X},\mathbf{Y}) = \mathcal{N}(\mathbf{w};\boldsymbol{\mu},\boldsymbol{\Sigma}) \Rightarrow$ we can sample from posterior
  - No observation : $p(\mathbf{w}/\mathbf{X},\mathbf{Y}) = p(\mathbf{w})$
  - $N \geq 1$: prior biased by data likelihood
  - Ex : $p(\mathbf{w}|\mathbf{x}_0,\mathbf{y}_0) \propto p(\mathbf{w})p(\mathbf{y}_0|\mathbf{x}_0,\mathbf{w})$
  - $p(\mathbf{w}|(\mathbf{x}_0,\mathbf{y}_0),(\mathbf{x}_1,\mathbf{y}_1)) \propto p(\mathbf{w}|\mathbf{x}_0,\mathbf{y}_0)p(\mathbf{y}_1|\mathbf{x}_1,\mathbf{w}) \propto p(\mathbf{w})p(\mathbf{y}_0|\mathbf{x}_0,\mathbf{w})p(\mathbf{y}_1|\mathbf{x}_1,\mathbf{w})$ ....



Bayesian Linear Regression : Posterior Sampling



0 data points are observed.

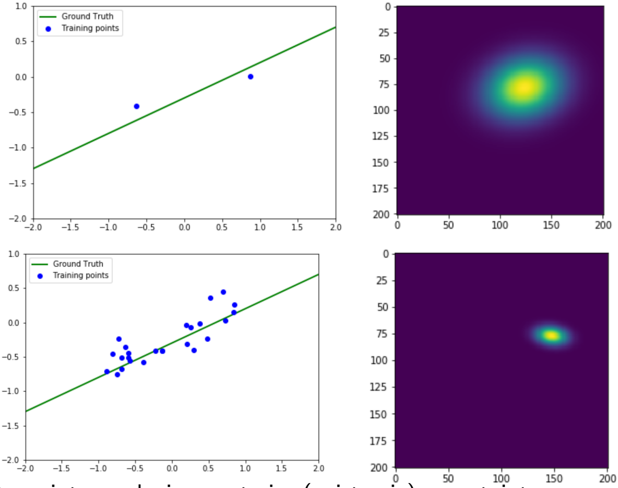
1 data point is observed.

2 data points are observed.

20 data points are observed.

Bayesian Linear Regression : Posterior Sampling

Practical session : compute posterior



- More data points : reducing posterior (epistemic) uncertainty
- $N \to \infty$ posterior uncertainty $\Leftrightarrow$ aleatoric uncertainty

Bayesian Linear Regression : Predictive Distribution

$p(\mathbf{w}|\mathcal{D},\alpha,\beta) \Rightarrow$ compute predictive distribution by marginalizing over $\mathbf{w}$:

- $p(y|\mathbf{x}^*,\mathcal{D},\alpha,\beta) = \int p(y|\mathbf{x}^*,\mathbf{w},\beta)p(\mathbf{w}|\mathcal{D},\alpha,\beta)dw$
  - $p(y|\mathbf{x}^*,\mathbf{w},\beta) = \mathcal{N}(y;\mathbf{\Phi}(\mathbf{x}^*)^T\mathbf{w},\beta^{-1})$: likelihood
  - $p(\mathbf{w}|\mathcal{D},\alpha,\beta) = \mathcal{N}(\mathbf{w};\boldsymbol{\mu},\mathbf{\Sigma})$: $\mathbf{w}$ posterior
    - $\mathbf{\Sigma}^{-1} = \alpha \boldsymbol{I} + \beta\mathbf{\Phi}^T\mathbf{\Phi}$
    - $\boldsymbol{\mu} = \beta\mathbf{\Sigma}\mathbf{\Phi}^T\mathbf{Y}$
- $p(y|\mathbf{x}^*,\mathcal{D},\alpha,\beta)$: convolution of two Gaussians $\Rightarrow$ Gaussian
  - Mean of predictive distribution $\mu^T\mathbf{\Phi}(\mathbf{x}^*)$
  - Variance of predictive distribution $\sigma^2_{pred}(\mathbf{x}^*) = \frac{1}{\beta} + \mathbf{\Phi}(\mathbf{x}^*)^T\mathbf{\Sigma}\mathbf{\Phi}(\mathbf{x}^*)$

$$\boxed{p(y|\mathbf{x}^*,\mathcal{D},\alpha,\beta) = \mathcal{N}(y;\mu^T\mathbf{\Phi}(\mathbf{x}^*),\frac{1}{\beta} + \mathbf{\Phi}(\mathbf{x}^*)^T\mathbf{\Sigma}\mathbf{\Phi}(\mathbf{x}^*))}$$

Bayesian Linear Regression : Predictive Distribution

$$\boxed{p(y|\mathbf{x}^*, \mathcal{D}, \alpha, \beta) = \mathcal{N}(y; \mu^T \mathbf{\Phi}(\mathbf{x}^*), \frac{1}{\beta} + \mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*))}$$

- $\sigma^2_{pred}(\mathbf{x}^*) = \frac{1}{\beta} + \mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*)$
- β is actually our noise representation (**aleatoric**)
- $\mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*)$ is uncertainty over parameters $\mathbf{w}$ (**epistemic**)
- $\sigma^2_{pred}(\mathbf{x}^*)$ actually depends on N, $\sigma^2_{pred}(\mathbf{x}^*, N)$
  - $\sigma^2_{pred}(\mathbf{x}^*, N+1)$ ¡ $\sigma^2_{pred}(\mathbf{x}^*, N)$
  - $\lim_{N \to \infty} \mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*) = 0$: epistemic uncertainty removed by adding data samples

Bayesian Linear Regression : Predictive Distribution

$$p(y|\mathbf{x}^*, \mathcal{D}, \alpha, \beta) = \mathcal{N}(y; \mu^T \mathbf{\Phi}(\mathbf{x}^*), \sigma^2_{pred}(\mathbf{x}^*))$$

- $\sigma^2_{pred}(\mathbf{x}^*) = \beta^{-1} + \mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*)$
- $\mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*)$ is uncertainty over parameters $\mathbf{w}$ **(epistemic)**
- **Practical session :** in case of 1D inputs & outputs, *i.e.* $x_i \in \mathbb{R}$, $\mathbf{X} \in \mathbb{R}^{N \times 1}$, $\mathbf{X} \in \mathbb{R}^{N \times 1}$, $\mathbf{w} \in \mathbb{R}^2$, $\mathbf{\Phi} \in \mathbb{R}^{N \times 2}$:

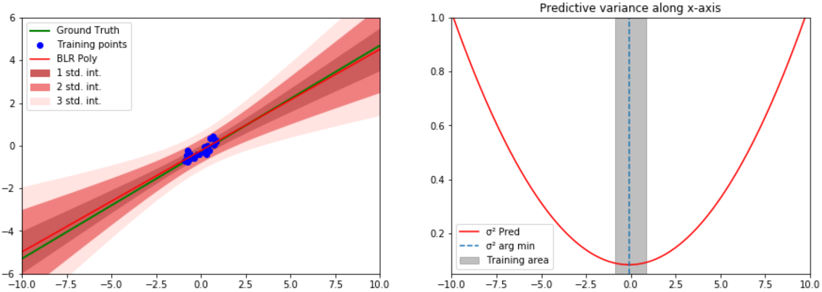
$$\mathbf{\Sigma}^{-1} = \alpha \boldsymbol{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi} = \begin{pmatrix} \alpha + \beta N & \beta \mathbf{1}^T \mathbf{X} \\ \beta \mathbf{1}^T \mathbf{X} & \alpha + \beta \mathbf{X}^T \mathbf{X} \end{pmatrix}$$

$\Rightarrow$ $\mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*)$ **Increases when $\mathbf{x}^*$ far from training data**

- $\mathbf{x}^*_{min} = \frac{\sum_i x_i}{N + \alpha / \beta}$

Bayesian Linear Regression : Predictive Distribution

Practical session : predictive distribution and uncertainty



Bayesian Linear Regression

- Note on MAP estimate :

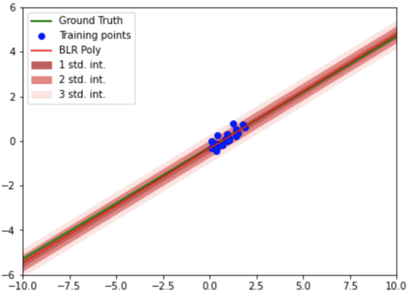
$$
\begin{aligned}
\mathbf{w}_{MAP} &= \arg\min_{\mathbf{w}} - \sum_{n=1}^{N} \log p(\mathbf{w}|\mathbf{x}_n, y_n, \beta, \alpha) \\
&= \arg\min_{\mathbf{w}} - \sum_{n=1}^{N} \log p(y_n|\mathbf{x}_n, \mathbf{w}, \beta, \alpha) - \log p(\mathbf{w}|\alpha) \\
&= \arg\min \frac{\beta}{2} \sum_{i=1}^{N} ||y_n - f^{\mathbf{w}}(\mathbf{x}_n)||^2 + \frac{\alpha}{2} \mathbf{w}^T \mathbf{w}
\end{aligned}
$$

$\Rightarrow$ **adding a Gaussian prior with precision on weights α acts like L_2 regularisation (weight decay) with $\lambda = \alpha/\beta$**

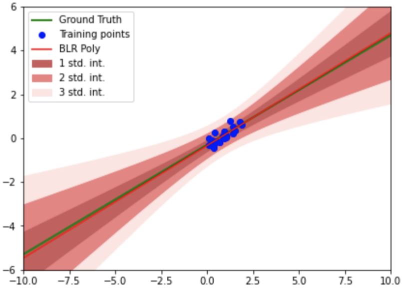
Bayesian Linear Regression : Predictive Distribution

Prediction distribution $\neq$ likelihood at $w = w_{MAP}$

- **Likelihood at** $w = w_{MAP}$: $p(y|\mathbf{x}^*, w_{MAP}) = \mathcal{N}(y; \mu^T \mathbf{\Phi}(\mathbf{x}^*), \sigma^2))$
  - $\sigma^2 = Cte \quad \forall \mathbf{x}^*$
- **Prediction distribution :** $p(y|\mathbf{x}^*, \mathcal{D}, \alpha, \beta) = \int p(y|\mathbf{x}^*, \mathbf{w}, \beta) p(\mathbf{w}|\mathcal{D}, \alpha, \beta) dw = \mathcal{N}(y; \mu^T \mathbf{\Phi}(\mathbf{x}^*), \sigma^2_{pred}(\mathbf{x}^*))$
  - $\sigma^2_{pred} = f(\mathbf{x}^*) = \beta^{-1} + \mathbf{\Phi}(\mathbf{x}^*)^T \mathbf{\Sigma} \mathbf{\Phi}(\mathbf{x}^*)$



$p(y|\mathbf{x}^*, w_{MAP})$

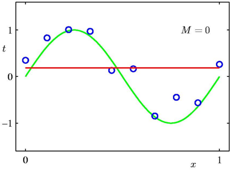


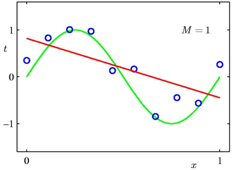
$p(y|\mathbf{x}^*, \mathcal{D}, \alpha, \beta)$

Non-Linear Regression

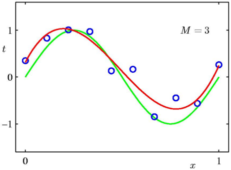
- Linear regression : limited in many datasets
- Non-linear extension by designing explicit non-linear feature maps $\mathbf{\Phi}$
  - Ex : Polynomial regression for 1D input, *i.e.* $x_i \in \mathbb{R}$:

$$\mathbf{\Phi} = \begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^M \\ 1 & x_2 & x_2^2 & \dots & x_2^M \\ \dots & \dots & \dots & \dots & \\ 1 & x_N & x_N^2 & \dots & x_N^M \end{pmatrix} \qquad \mathbf{Y} = \mathbf{\Phi} \mathbf{w} + \boldsymbol{\varepsilon} \qquad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_1 & \dots & \varepsilon_N \end{pmatrix}^T, \ \varepsilon_i \sim \mathcal{N}(0, \sigma^2)$$

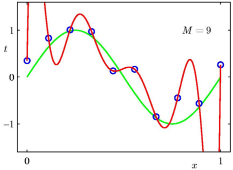




← Poor representations of $\sin(2\pi x)$



← Best Fit to $\sin(2\pi \mathrm{x})$



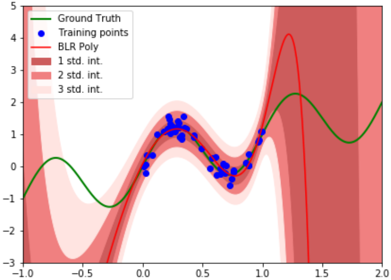
Over Fit
Poor representation of $\sin(2\pi \mathrm{x})$

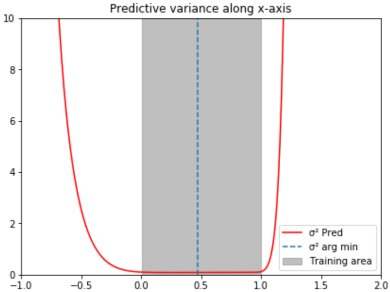
Bayesian Polynomial Regression

- Polynomial regression for 1D input, *i.e.* $x_i \in \mathbb{R}$:

$$\mathbf{\Phi} = \begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^M \\ 1 & x_2 & x_2^2 & \dots & x_2^M \\ \dots & \dots & \dots & \dots & \\ 1 & x_N & x_N^2 & \dots & x_N^M \end{pmatrix} \qquad \mathbf{Y} = \mathbf{\Phi}\mathbf{w} + \boldsymbol{\varepsilon} \qquad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_1 & \dots & \varepsilon_N \end{pmatrix}^T, \ \varepsilon_i \sim \mathcal{N}(0, \sigma^2)$$

- Apply Bayesian linear regression in non-linear feature space $\mathbf{\Phi}$
  - Same closed-form solution for posterior and predictive distribution in $\mathbf{\Phi}$
- Practical session : regression for $f(x) = x + sin(2\Pi x)$, $M = 10$, $\alpha = 0.05$



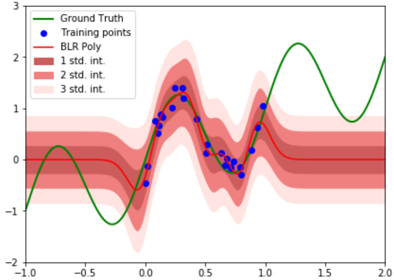


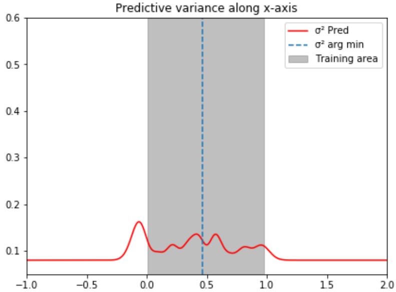
RBF Gaussian Regression

- Gaussian regression for 1D input, *i.e.* $x_i \in \mathbb{R}$, $\Phi_j(x_i) = exp\left(-\frac{(x_i - \mu_j)^2}{2s^2}\right)$:

$$\boldsymbol{\Phi} = \begin{pmatrix} \Phi_1(x_1) & \Phi_2(x_1) & \dots & \Phi_M(x_1) \\ \dots & \dots & \dots & \dots \\ \Phi_1(x_N) & \Phi_2(x_N) & \dots & \Phi_M(x_N) \end{pmatrix} \quad \mathbf{Y} = \boldsymbol{\Phi}\mathbf{w} + \varepsilon, \; \varepsilon_i \sim \mathcal{N}(0, \sigma^2)$$

- Apply Bayesian linear regression in non-linear feature space $\boldsymbol{\Phi}$





- Practical session : issue with localized features, epistemic uncertainty $\boldsymbol{\Phi}(\mathbf{x}^*)^T \boldsymbol{\Sigma} \boldsymbol{\Phi}(\mathbf{x}^*) \rightarrow 0$ far from trainig data (μ_j)

Outline

Beyond Bayesian Linear Regression

- Posterior distribution for parameters $\mathbf{w}$: $p(\mathbf{w}|\mathbf{X},\mathbf{Y}) \propto p(\mathbf{Y}|\mathbf{X},\mathbf{w})p(\mathbf{w})$
- Predictive distribution $p(y|\mathbf{x}^*,\mathcal{D}) = \int p(y|\mathbf{x}^*,\mathbf{w})p(\mathbf{w}|\mathcal{D})dw$, $(\mathbf{X},\mathbf{Y}) := \mathcal{D}$
- **Closed form for posterior $p(\mathbf{w}|\mathcal{D})$ and predictive distribution $p(y|\mathbf{x}^*,\mathcal{D})$: more the exception than the rule !**
- Slightly more complicated models : no closed form solution
  - Bayesian Logistic Regression
    - Simplest linear classification model
    - Likelihood not Gaussian
  - Neural network with one hidden layer in general
    - No closed form for regression and classification
  - And of course deep neural networks

Approximate Inference

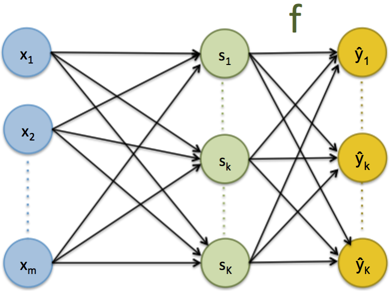
No analytical expression for posterior $p(\mathbf{w}|\mathcal{D})$ and $p(y|\mathbf{x}^*, \mathcal{D})$ in general

$\Rightarrow$ **Approximation nedded !**

- **Gaussian approximation for $p(\mathbf{w}|\mathcal{D})$**
  - **Ex : Laplace approximation** [MacKay, 1992]
  - Historically used for bayesian logistic regression
- **Monte Carlo methods** : sampling to directly evaluate integral $p(y|\mathbf{x}^*, \mathcal{D})$
  - **Metropolis-Hasting, Hamiltonian Monte Carlo** [Neal, 1996], **Expectation propagation** [Hernandez-Lobato and Adams, 2015, Jylänki et al., 2014]
- **Variational inference** [Hinton and van Camp, 1993, Graves, 2011, Blundell et al., 2015] : convert integration into optimization
  - Minimize KL divergence between $p(\mathbf{w}|\mathcal{D})$ and a proposed parametric function

Outline

Bayesian Logistic Regression (BLR)



- $\mathbf{s}_i = \mathbf{W}\mathbf{x}_i$
- Multi-class : $p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{w}) = \hat{\mathbf{y}}_\mathbf{i}$
  - $\hat{y}_{i,k} = \frac{exp(s_i)}{\sum\limits_k exp(s_k)}$
- Binary case : $p(\mathbf{y}_i = 1|\mathbf{x}_i, \mathbf{w}) = \sigma(s_i)$
  - σ sigmoid
  - $p(\mathbf{y}_i = -1|\mathbf{x}_i, \mathbf{w}) = 1 - \sigma(s_i)$

$$p(\mathbf{w}|\mathbf{X}, \mathbf{Y}) \propto p(\mathbf{Y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

- $p(\mathbf{Y}|\mathbf{X}, \mathbf{w}) = \prod\limits_{i=1}^{N} p(\mathbf{y}_i = 1|\mathbf{x}_i, \mathbf{w})$ not Gaussian anymore !

$\Rightarrow$ **no closed-form on posterior distribution $p(\mathbf{w}|\mathbf{X}, \mathbf{Y})$!**

Bayesian Logistic Regression training (MAP)

$$\boldsymbol{w}_{\text{MAP}} = arg\max_{\boldsymbol{w}} p(\mathbf{X}, \mathbf{Y}|\boldsymbol{w})p(\boldsymbol{w}) = arg\max_{\boldsymbol{w}} \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n, \boldsymbol{w})p(\boldsymbol{w})$$

$$= arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} -log\left(p(y_n|\boldsymbol{x}_n, \boldsymbol{w})\right) - log\left(p(\boldsymbol{w})\right)$$

- Gaussian prior : $p(\boldsymbol{w}) = \mathcal{N}(\mathbf{w}; 0, \sigma_0^2 I)$;
- MAP with binary prediction :

$$\boldsymbol{w}_{\text{MAP}} = arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} \left(-y_n \log \sigma(\boldsymbol{w}^T \boldsymbol{x}_n + b) - (1 - y_n) \log(1 - \sigma(\boldsymbol{w}^T \boldsymbol{x}_n + b)) + \frac{1}{2\sigma_0^2} ||\boldsymbol{w}||_2^2 \right)$$

  - Gaussian prior $\Leftrightarrow$ weight decay

Bayesian Logistic Regression training (MAP)

$$\boldsymbol{w}_{\text{MAP}} = arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} -log\left(p(y_n|\boldsymbol{x}_n, \boldsymbol{w})\right) + \frac{1}{2\sigma_0^2}||\boldsymbol{w}||_2^2$$

- $\boldsymbol{w}_{\text{MAP}}$ with gradient descent
- We want to estimate predictive distribution :

$$p(\mathbf{y} = 1|\boldsymbol{x}^*, \mathcal{D}) = \int p(\mathbf{y} = 1|\boldsymbol{x}, \boldsymbol{w})p(\boldsymbol{w}|\mathcal{D})d\boldsymbol{w}$$

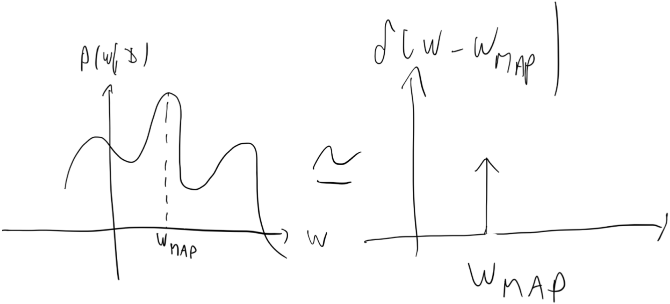
Bayesian Logistic Regression training (MAP)

$$\boldsymbol{w}_{\mathrm{MAP}} = arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} \left(-y_n \log \sigma(\boldsymbol{w}^T \boldsymbol{x}_n + b) - (1 - y_n) \log(1 - \sigma(\boldsymbol{w}^T \boldsymbol{x}_n + b)) + \frac{1}{2\sigma_0^2} ||\boldsymbol{w}||_2^2 \right)$$

- $\boldsymbol{w}_{\mathrm{MAP}}$ with gradient descent
- We want to estimate predictive distribution :

$$p(\mathbf{y} = 1 | \boldsymbol{x}^*, \mathcal{D}) = \int p(\mathbf{y} = 1 | \boldsymbol{x}, \boldsymbol{w}) p(\boldsymbol{w} | \mathcal{D}) d\boldsymbol{w}$$

  - Need full posterior distribution $p(\mathbf{w}|\mathbf{X}, \mathbf{Y})$, but posterior intractable
  - $p(\mathbf{w}|\mathbf{X}, \mathbf{Y}) \approx \delta(\mathbf{w} - \boldsymbol{w}_{\mathrm{MAP}}) \Rightarrow p(\mathbf{y} = 1 | \boldsymbol{x}^*, \mathcal{D}) \approx p(y = 1 | \boldsymbol{x}, \boldsymbol{w}_{\mathrm{MAP}})$



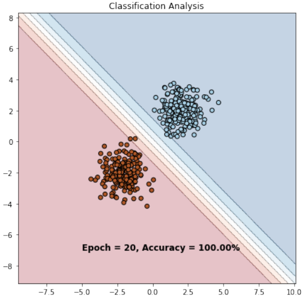
Bayesian Logistic Regression training (MAP)

$$\boldsymbol{w}_{\mathrm{MAP}} = arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} \left(-y_n \log \sigma(\boldsymbol{w}^T \boldsymbol{x}_n + b) - (1-y_n)\log(1-\sigma(\boldsymbol{w}^T \boldsymbol{x}_n + b)) + \frac{1}{2\sigma_0^2}||\boldsymbol{w}||_2^2 \right)$$

- $\boldsymbol{w}_{\mathrm{MAP}}$ with gradient descent
- Recap : we want to estimate predictive distribution :

$$p(\mathbf{y}=1|\boldsymbol{x}^{*},\mathcal{D}) = \int p(\mathbf{y}=1|\boldsymbol{x},\boldsymbol{w})p(\boldsymbol{w}|\mathcal{D})d\boldsymbol{w}$$

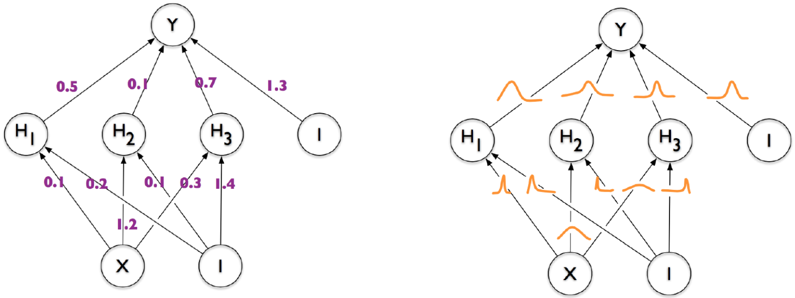
  - Need full posterior distribution $p(\mathbf{w}|\mathbf{X},\mathbf{Y})$, but posterior intractable
  - $p(\mathbf{w}|\mathbf{X},\mathbf{Y}) \approx \delta(\mathbf{w}-\boldsymbol{w}_{\mathrm{MAP}}) \Rightarrow p(\mathbf{y}=1|\boldsymbol{x}^{*},\mathcal{D}) \approx p(y=1|\boldsymbol{x},\boldsymbol{w}_{\mathrm{MAP}})$



- $p(\mathbf{w}|\mathbf{X},\mathbf{Y}) \approx \delta(\mathbf{w}-\boldsymbol{w}_{\mathrm{MAP}})$: very coarse approximation :
- Uncertainty does not increase far from training data
- Need for more accurate approximations

Outline

Bayesian Neural Networks (BNN)



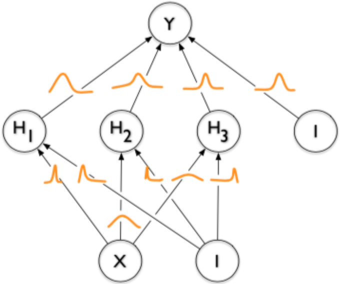
Credit : [Blundell et al., 2015]

- $\boxed{\text{Standard NN : } \mathbf{y}_i = f^{\mathbf{w}}(\mathbf{x}_i), \textbf{ Bayesian NN : } p(\mathbf{y}_i|\mathbf{x}_i, \mathcal{D})}$
  - Define prior over weights $p(\mathbf{w})$, *e.g.* $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|0, \alpha^{-1}\mathcal{I})$ (point estimate for bias)
    - In practice, typically separate variance $\sigma^2 = \alpha^{-1}$ for each layer
  - Define likelihood, $p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{w})$, *e.g.* for regression $p(y_i|\mathbf{x}_i, \mathbf{w}) = \mathcal{N}(y_i; f^w(\mathbf{x}_i), \beta^{-1})$
  - **<u>Goal :</u> compute posterior** $p(\mathbf{w}|\mathbf{X}, \mathbf{Y}) = \prod_{i=1}^{N} p(\mathbf{w}|\mathbf{x}_i, \mathbf{y}_i, \beta) \propto p(\mathbf{w}) \prod_{i=1}^{N} p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{w})$

Bayesian Neural Networks (BNN)

$$p(\mathbf{w}|\mathbf{X}, \mathbf{Y}) \propto p(\mathbf{w}) \prod_{i=1}^{N} p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{w})$$

- **With Bayesian Neural networks, even with :**
  - Gaussian prior $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|0, \alpha^{-1}\mathcal{I})$
  - Gaussian likelihood, *e.g.* regression $p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{w}) = \mathcal{N}(y_i; f^w(\mathbf{x}_i), \beta^{-1})$
  - Posterior $p(\mathbf{w}|\mathbf{X}, \mathbf{Y}, \beta) \propto p(\mathbf{w}) \prod_{i=1}^{N} p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{w})$ **is NOT Gaussian ! !**
- **Non-linear dependence of $f^w(\mathbf{x})$ on $\mathbf{w}$!**
- RECAP :
  - $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_x)$
  - $p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}|A\mathbf{x} + b, \boldsymbol{\Sigma}_y)$
    - Linear depedence $A\mathbf{x} + b$ required
  - Then : $p(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{x|\mathbf{y}}, \boldsymbol{\Sigma}_{x|\mathbf{y}})$
    - Not true for BNNs !



Credit : [Blundell et al., 2015]

Posterior Inference : MCMC Sampling

The true predictive distribution $p(y|\mathbf{x}^*, \mathcal{D})$ cannot be evaluated analytically

$$p(y|\mathbf{x}^*, \mathcal{D}) = \int p(y|\mathbf{x}^*, \mathbf{w}) p(\mathbf{w}|\mathcal{D}) dw$$

- Monte Carlo estimation of the intergral :

$$p(y|\mathbf{x}^*, \mathcal{D}) \approx \frac{1}{S} \sum_{s=1}^{S} p(y|\mathbf{x}^*, \mathbf{w}^s) \qquad \mathbf{w}^s \sim p(\mathbf{w}|\mathcal{D})$$

- Can't sample exactly from $p(\mathbf{w}|\mathcal{D})$, **BUT approximate sampling using Markov chain Monte Carlo (MCMC) possible !**
  - Metropolis-Hasting (MH), Hamiltonian Monte Carlo (HMC) [Neal, 1996]
- **Works well, accurate posterior inference in BNNs**
- **Main drawback : does not scale to large datasets**
  - **Computing likelihood for MH/HMC acceptance step requires the whole dataset**

Variational Inference (VI)

The true posterior $p(\mathbf{w}|\mathbf{X},\mathbf{Y})$ cannot usually be evaluated analytically

- Defining an **approximating variational distribution** $q_{\boldsymbol{\theta}}(\mathbf{w})$, parameterized by $\boldsymbol{\theta}$
- **Minimizing its KL divergence with the true posterior** :

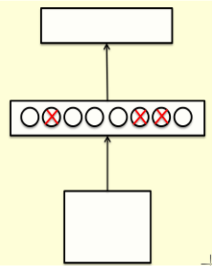
$$KL(q_{\boldsymbol{\theta}}(\mathbf{w})||p(\mathbf{w}|\mathbf{X},\mathbf{Y})) = \int q_{\boldsymbol{\theta}}(\mathbf{w}) \log \frac{q_{\boldsymbol{\theta}}(\mathbf{w})}{p(\mathbf{w}|\mathbf{X},\mathbf{Y})} d\mathbf{w}$$

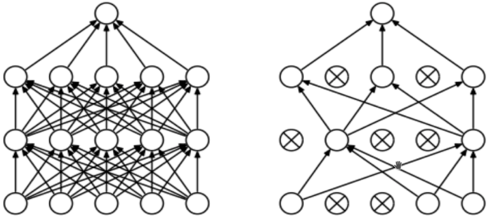
- **Computing approximate predictive distribution :** $p(\mathbf{w}|\mathbf{X},\mathbf{Y}) \Leftarrow q_{\boldsymbol{\theta}^*}(\mathbf{w})$:

$$p(\mathbf{y}|\mathbf{x}^*,\mathbf{X},\mathbf{Y}) \approx \int p(\mathbf{y}|x^*,\mathbf{w}) q_{\boldsymbol{\theta}^*}(\mathbf{w}) d\mathbf{w}$$

Dropout [Hinton et al., 2012]

- Randomly omit each hidden unit with probability p, *e.g.* $p = 0.5$
- **Regularization technique**, limits over-fitting (better generalization)
  - Prevent co-adaptation
  - May be viewed as averaging over many NN
  - Slower convergence





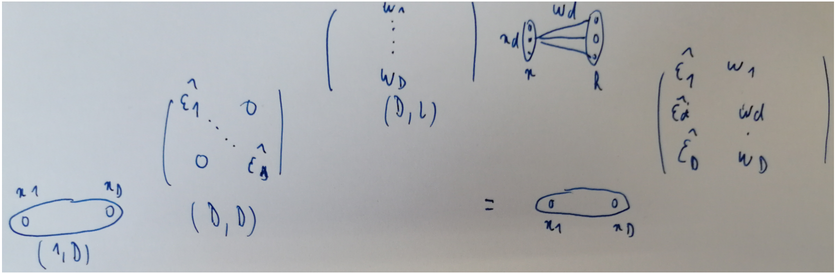
Standard Neural Net

After applying dropout.

Credits: Geoffrey E. Hinton, NIPS 2012

Dropout as a variational inference [Gal, 2016]

- Input $\mathbf{x} \in \mathbb{R}^{D}$ [a], latent vector $\mathbf{h} \in \mathbb{R}^{L}$
  - First layer : $\mathbf{h} = \sigma(\mathbf{x}\mathbf{W_1})$, σ non-linearity
- **Dropout sampling :** in input : $\mathbf{x} \odot \hat{\varepsilon}$
  - $\hat{\varepsilon} = \{\hat{\varepsilon}_i^1\}_{i\in\{1;D\}}\ \varepsilon_i \sim Bernoulli(1-p)$
  - First layer : $\mathbf{h} = \sigma((\mathbf{x} \odot \hat{\varepsilon})\mathbf{W_1})$
    - $(\mathbf{x}\,\mathrm{diag}(\hat{\varepsilon}))\mathbf{W_1} = \mathbf{x}(\,\mathrm{diag}(\hat{\varepsilon})\mathbf{W_1}) = \mathbf{x}\hat{\mathbf{W}}_\mathbf{1}$
    - Randomly setting to 0 rows of $\mathbf{W_1}$ (size $((D, L))$ with probability p



a. dimension (1,D)

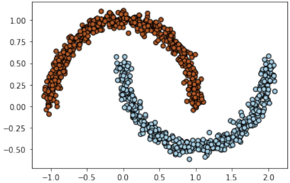
Dropout as a variational inference [Gal, 2016]

- **Illustration : dropout for a 2 layer NN** (1 hidden), $\epsilon_i \sim Bernoulli(1-p_i)$:
  - $\boxed{\mathbf{h_1} = \sigma(\hat{\mathbf{x}}\mathbf{W_1}) = \sigma(\mathbf{x}\hat{\mathbf{W}}_\mathbf{1})}$, $\hat{\mathbf{W}}_1 = \text{diag}(\hat{\epsilon_1})\mathbf{W_1}$
  - $\boxed{\hat{\mathbf{y}} =: f^{\hat{\mathbf{W}}_1, \hat{\mathbf{W}}_2}(\mathbf{x}) = \hat{\mathbf{h_1}}\mathbf{W_2} = \mathbf{h_1}\hat{\mathbf{W}}_\mathbf{2}}$, $\hat{\mathbf{W}}_2 = \text{diag}(\hat{\epsilon_2})\mathbf{W_2}$ - $\hat{\mathbf{W}} = \{\hat{\mathbf{W}}_\mathbf{1}; \hat{\mathbf{W}}_\mathbf{2}\}$
- **MC Dropout sampling :** $\frac{1}{S}\sum_{s\in S} p(\mathbf{y}_i|f^{\hat{\mathbf{W}}}(\mathbf{x}_i)) \approx \int p(\mathbf{y}|f^{\mathbf{W}}(\mathbf{x}^*)q(\mathbf{W})d\mathbf{w}$
  - $\forall$ layer $l \in \{1; L\}$, $\mathbf{W}_l$ random variable : $\mathbf{W}_l \sim q(\mathbf{W}_l) = g(\mathbf{M}_l, \varepsilon_l) = \text{diag}(\boldsymbol{\varepsilon_l})\mathbf{M}_l$
    - $\varepsilon_{l,i} \sim Bernoulli(1-p_l)$, $\mathbf{M}_l$ deterministic parameters
  - $q_\mathbf{M}(\mathbf{W}) = \prod_{l=1}^{M} q_{\mathbf{M_l}}(\mathbf{W}_l)$
- **Big result** (see [Gal, 2016]) : **training NN with dropout** $\Leftrightarrow$ **training BNN with variational posterior approximation** $q_\mathbf{M}(\mathbf{W})$ (and some prior $p(\mathbf{W})$)
  - $\mathbf{M} = \{\mathbf{M}_l\}_{l\in\{1;L\}}$ variational parameters
- **MC dropout :** sampling several passes with dropout $\Leftrightarrow$ **performing MC approximate inference with variational posterior** $q_\mathbf{M}(\mathbf{W})$

$$\boxed{\frac{1}{S}\sum_{s\in S} p(\mathbf{y}_i|f^{\hat{\mathbf{W}}}(\mathbf{x}_i)) \approx \int p(\mathbf{y}|f^{\mathbf{W}}(\mathbf{x}^*)q(\mathbf{W})d\mathbf{w} \approx p(y|\mathbf{x}^*, \mathbf{X}, \mathbf{Y})}$$

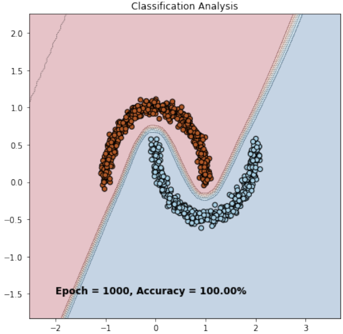
Application : MC dropout for predictive distribution

- MC dropout for non-linear classification

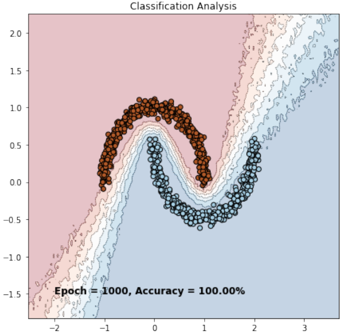


- As for BLR : $p(y=1|\mathbf{x}^*, \mathcal{D}) \approx \sum_{s=1}^{S} f_{\mathbf{w}^s}(\mathbf{x}^*)$, $\mathbf{w}^s \sim q(\mathbf{W})$

Deterministic NN



Bayesian NN (MC dropout)



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