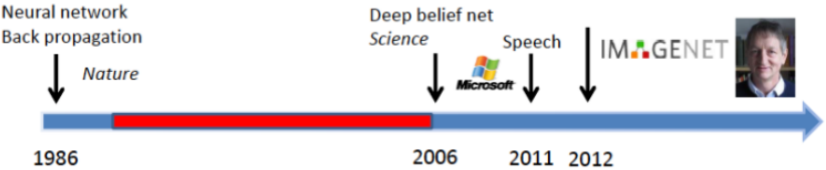
Sorbonne Université, Computer Science Master
Données, Apprentissage et Connaissances (DAC)
Bayesian Deep Learning

Nicolas Thome
Sorbonne Université
ISIR Lab - Machine Learning Team (MLIA)

Deep Learning Success since 2010

- 90's / 2000's: difficult to train large deep models on existing databases

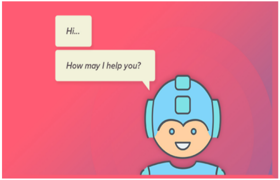


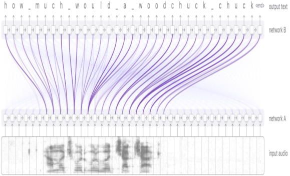
- **ILSVRC'12: the deep revolution**
  ⇒ outstanding success of ConvNets [Krizhevsky et al., 2012]

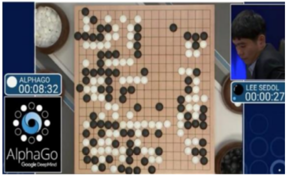
Rank	Name	Error rate	Description
1	**U. Toronto**	0.15315	Deep learning
2	U. Tokyo	0.26172	Hand-crafted features and learning models. Bottleneck.
3	U. Oxford	0.26979	
4	Xerox/INRIA	0.27058	

Deep Learning everywhere since 2012

- Image classification, speech recognition
- chatbots, translation,
- Games, robotics

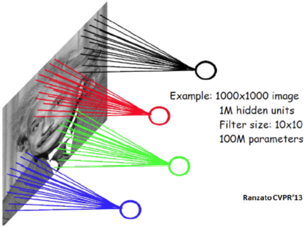


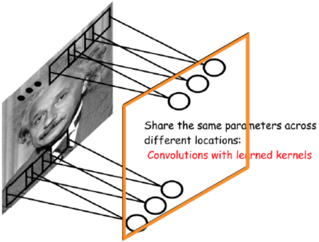




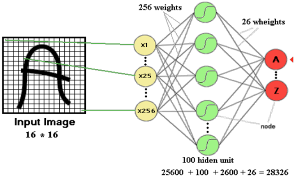
Convolutional Neural Networks (ConvNets)

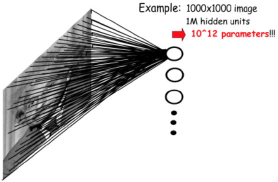
- **<u>ConvNets:</u>** sparse connectivity + shared weights





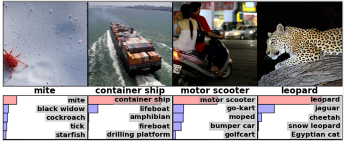
- **Local feature extraction ($\neq$ FCN)**
- Overcome parameter explosion for FCN on images



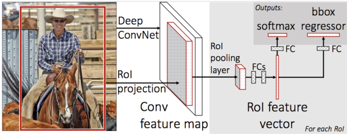


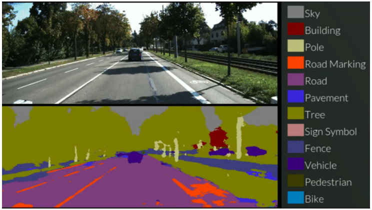
Deep Learning in Computer Vision

[*Krizhevsky*, 2012]



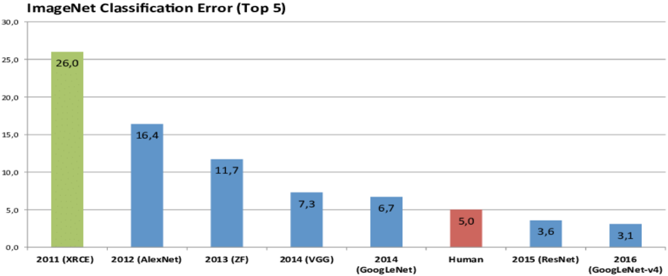
[*Girshick et al.* Fast R-CNN, 2015]





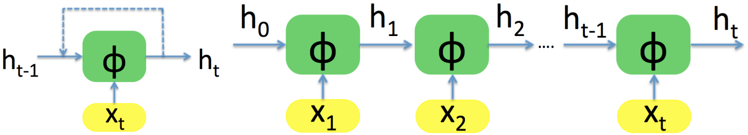
[*Kendall et al.* SegNet, 2015]

Brought significant improvements in multiple vision tasks



Recurrent Neural Networks (RNNs)

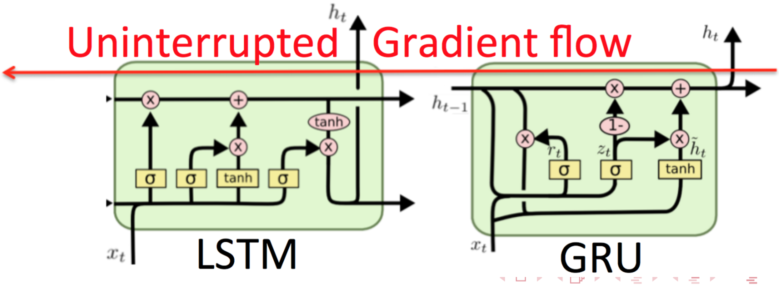
- **RNN Cell:** $h_t = \phi(x_t, h_{t-1}) = f(Ux_t + Wh_{t-1} + b_h)$ [Elman, 1990]
  - h_t: **network memory up to time t $\Rightarrow$ Sequence processing**



Folded RNN

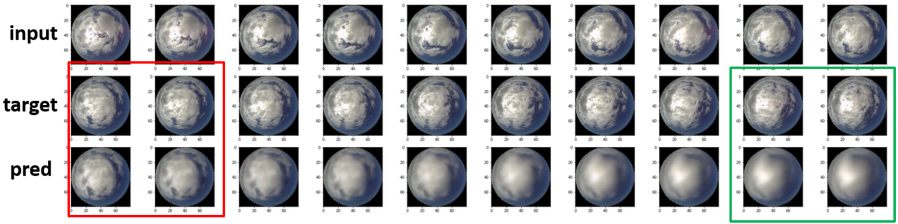
Unfolded RNN

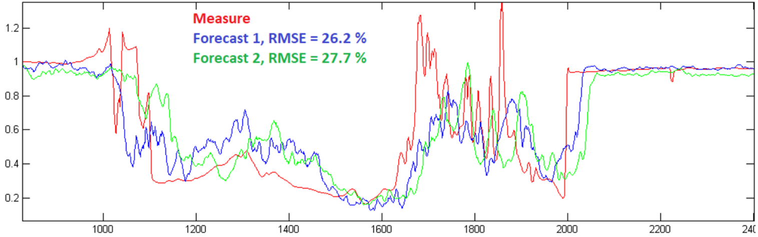
- **Specific architectures for vanishing gradients:**
  LSTM [Hochreiter and Schmidhuber, 1997], GRU [Cho et al., 2014]



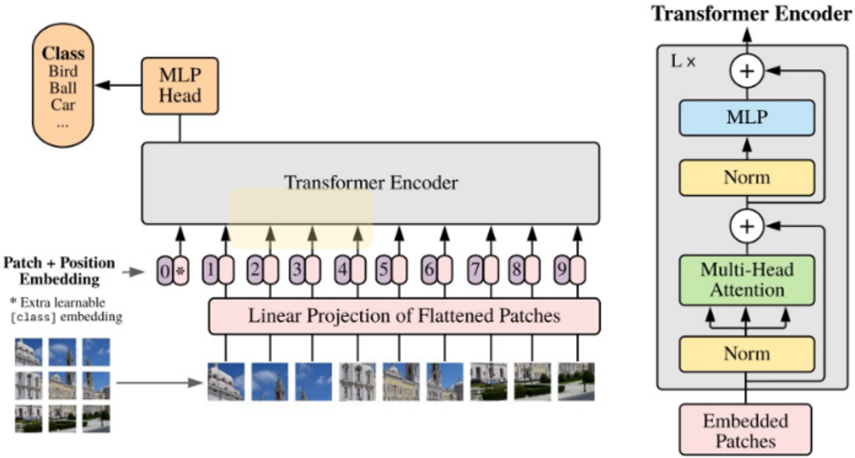
Deep Learning for Sequence Processing

- RNNs SOTA for many sequential decision making tasks: speech, translation, text/music generation, times series, etc
- Ex: video forecasting, *i.e.* prediction future frames





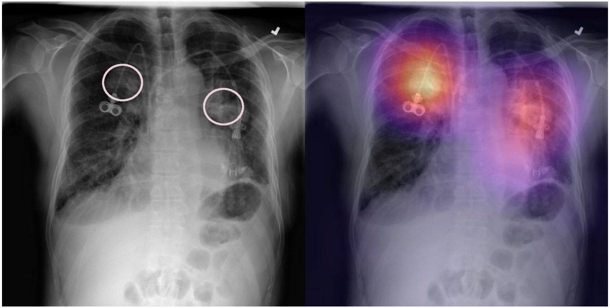
Vision Transformers (ViT)

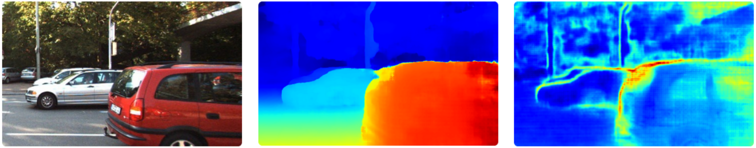


Robustness in Deep Learning

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

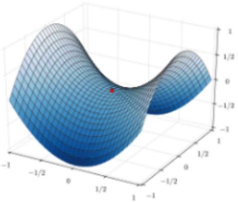
- Need for **performance certification in safety-critical applications: robustness**
  - Healthcare, autonomous steering, nuclear, defense, *etc*

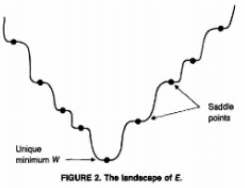


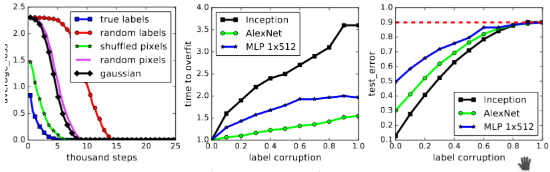


Performance certification

- **Formal understanding of deep learning:**
  - Understanding generalization performances with over-parameterized networks
  - Optimization, landscape loss function



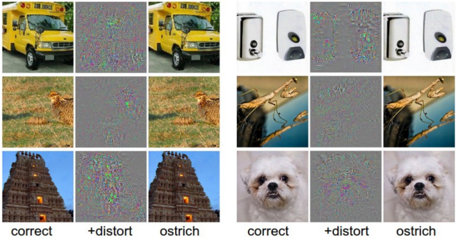




(a) learning curves (b) convergence slowdown (c) generalization error growth

Performance certification

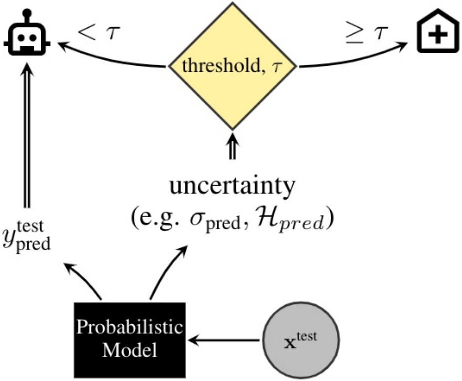
- **Stability of the decision function**, *e.g.* robustness to adversarial attacks



[Evtimov et al., 2017]

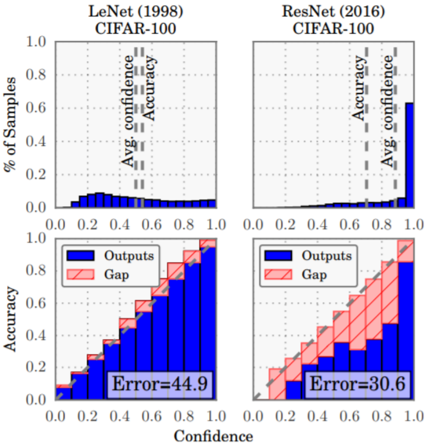
Performance certification

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



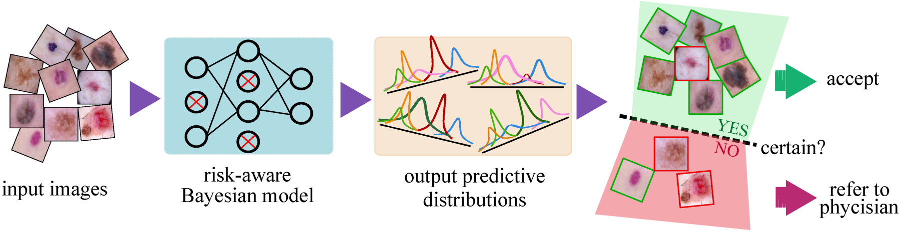
Performance certification

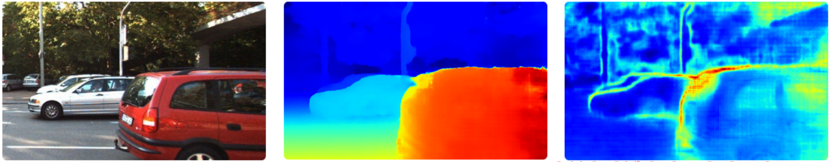
- **Reliable confidence / uncertainly estimation** of the decision process
  - Deep learning models overconfident, poor at this task [Guo et al., 2017]



Performance certification

- **Reliable confidence / uncertainly estimation** of the decision process
  - Crucial for deployment in healthcare / autonomous steering applications





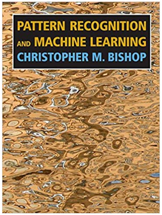
Robustness in Deep Learning

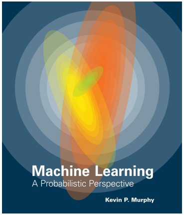
This course: 3 weeks on robust deep learning

`https://rdfia.github.io/`

1. Bayesian models and uncertainty estimation
   - Bayesian linear regression and extension to non-linear feature maps
2. Bayesian deep learning
   - Approximate posterior inference, variational approximation
   - Monte Carlo dropout
3. Application of uncertainty, other robustness issues
   - failure prediction and OOD detection

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





Outline

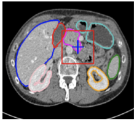
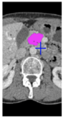
Type of uncertainties

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

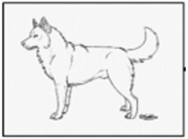
- *aleator* (lat.) = dice player
- **Noise inherent in the observations**, *i.e.* natural randomness.
- Cannot be reduced (need to change input/sensor), but can be estimated/learned
- Two (sub)-types of aleatoric uncertainty:
  1. **homoscedastic uncertainty**: stays constant for different input values,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

Type of uncertainties

Epistemic uncertainty

- *Episteme* (gr.): knowledge ⇒ **model uncertainty**
- Lack of knowledge about the generating process y (class) → input (image)



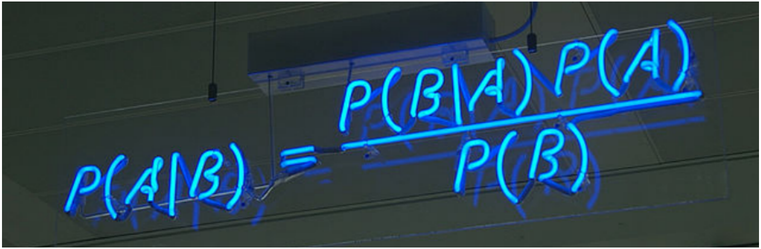
- **Main feature:** detects samples far from the training distribution
- Can be explained away given enough data
  - Epistemic uncertainty ↓ when number of data N (evidence) ↑
  - Epistemic uncertainty → 0 when $N \to \infty$

Outline

Bayesian Models

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

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

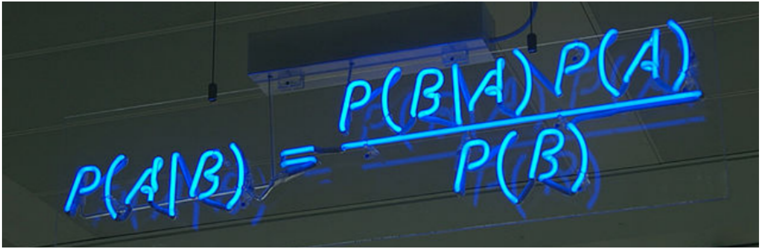


Bayesian Models

- **What we model:** $p(Y/X, w)$: likelihood and $p(w)$: prior knowledge
- **What we compute:** $p(w/X, Y) \propto p(Y/X, w)p(w)$ posterior
  biases prior $p(w)$ once data observed through likelihood $p(Y/w, X)$

How to estimate optimal w**?**

- **Maximum Likelihood (ML):** ignore (or assume uniform) prior
  $\Rightarrow$ find $\hat{w}$ s.t $p(Y/X, w)$ max
- **Maximum A Posteriori (MAP):** use prior $p(w)$
  $\Rightarrow$ find $\hat{w}$ s.t $p(w/X, Y)$ max



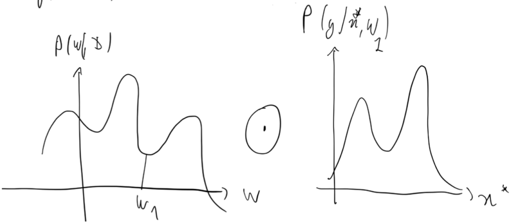
Bayesian Models & Uncertainty

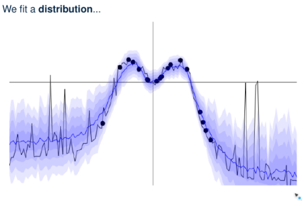
- From posterior $p(\mathrm{w}/\mathrm{X},\mathrm{Y}) \Rightarrow$ compute **predictive distribution** given new input x^* $(\forall y)$: $p(\mathrm{y}/\mathrm{x}^*,\mathrm{Y},\mathrm{X}) = \int p(\mathrm{y},\mathrm{w}/\mathrm{x}^*,\mathrm{Y},\mathrm{X})dw$

$$\boxed{p(\mathrm{y}/\mathrm{x}^*,\mathrm{Y},\mathrm{X}) = \int p(\mathrm{y}/\mathrm{x}^*,\mathrm{w})p(\mathrm{w}/\mathrm{X},\mathrm{Y})dw} = \mathbb{E}_{p(w|\mathcal{D})}[p(y|\mathrm{x}^*,\mathrm{w})]$$

  - **Naturally gives a measure of uncertainty**

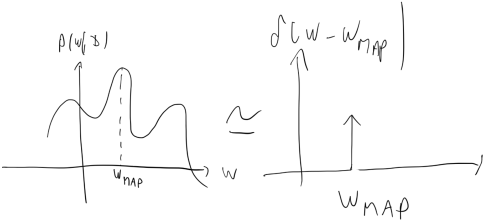
$P(y,w|x^*,D) \propto P(y|x^*,w)\,P(w|D)$



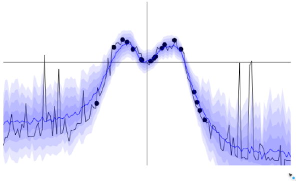


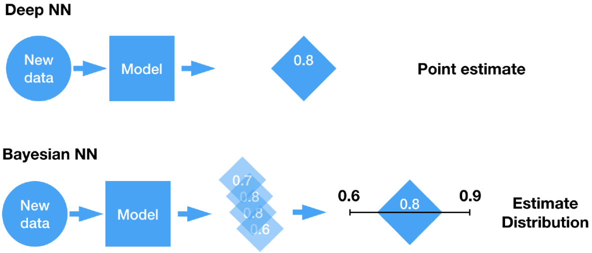
Bayesian vs deterministic models

- Deterministic models:
  $\boldsymbol{w}_{\mathrm{MAP}} = \mathit{arg}\max_{\boldsymbol{w}} p(w|\mathcal{D})$
- Only using $\boldsymbol{w}_{\mathrm{MAP}}$ for the posterior:
  $p(\mathrm{w}|\mathrm{X},\mathrm{Y}) \approx \delta(\mathrm{w} - \boldsymbol{w}_{\mathrm{MAP}})$
  $\Rightarrow p(\mathrm{y}|\boldsymbol{x}^*, \mathcal{D}) \approx p(y|\boldsymbol{x}, \boldsymbol{w}_{\mathrm{MAP}})$



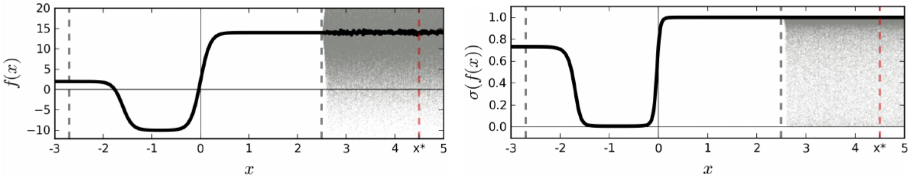
We fit a **distribution**...





Point-wise vs distribution modeling

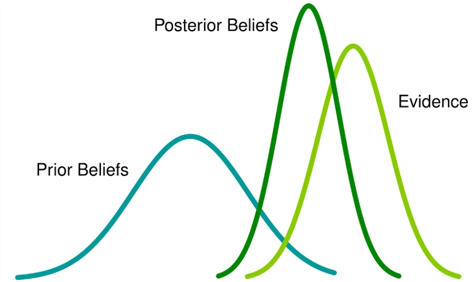
In binary classification, training a neural network to learn a function $f^w(x)$ (*e.g.* tanh) from a 1D dataset X=[-3,2], and apply Softmax to obtain probabilities.



- Point estimate through Softmax
  $\Rightarrow$ unjustified high confidence far from data: only model aleatoric uncertainty
- Distribution $p(y/x^*, Y, X)$ $\Rightarrow$ model epistemic uncertainty, should increase far from training data

Bayesian Models & Uncertainty

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



Outline

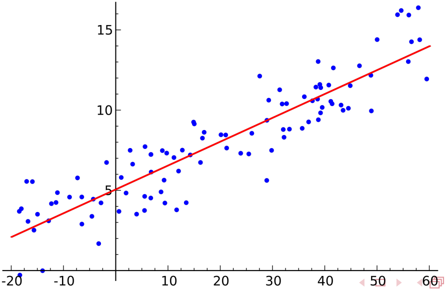
Probabilistic Linear Regression

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

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

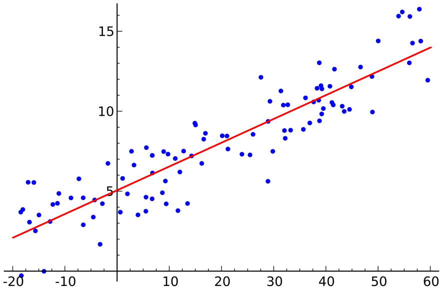
- $\boxed{\mathrm{Y} = \mathbf{\Phi}\mathrm{w} + \boldsymbol{\varepsilon}}$, $\boldsymbol{\varepsilon} \in \mathbb{R}^{N \times K}$, $\varepsilon_{i,k} \sim \mathcal{N}(0, \sigma^2)$
- $\mathrm{Y} \in \mathbb{R}^{N \times K}$, $\mathbf{\Phi} \in \mathbb{R}^{N \times (p+1)}$, $\mathrm{w} \in \mathbb{R}^{(p+1)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

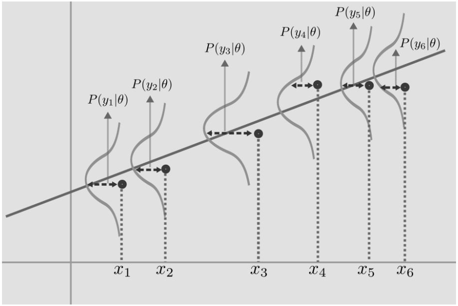
- Ex: scalar inputs and outputs $p = 1$, $K = 1 \Rightarrow \mathbf{\Phi} \in \mathbb{R}^{N \times 2}$, $\mathrm{w} \in \mathbb{R}^2$:



Probabilistic Linear Regression

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





- Trained with Maximum Likelihood (ML)
  - Examples assumed to be *i.i.d* (independent and identically distributed)

    $\Rightarrow p(\mathrm{Y}/\mathrm{X},\mathrm{w},\sigma) = \prod_{i=1}^{N} p(y_i/x_i,\mathrm{w},\sigma)$
  - MLE: $(\hat{\mathrm{w}},\hat{\sigma}) = \arg\max_{(\mathrm{w},\sigma)} p(\mathrm{X},\mathrm{Y}/\mathrm{w},\sigma) = \arg\min_{\mathrm{w},\sigma} -\sum_{i=1}^{N} log\left[p(\mathrm{y}_i/\mathrm{x}_i,\mathrm{w})\right]$
- MLE solution w: $\hat{\mathrm{w}} = \arg\min_{\mathrm{w}} C(\mathrm{w}) = \arg\min_{\mathrm{w}} \sum_{i=1}^{N} (\mathrm{y}_i - \mathbf{\Phi}_i^T \mathrm{w})^2$

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

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

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

Limits of MLE

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

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

- Choose **Prior**, *e.g.* $p(\mathrm{w}|\alpha) = \mathcal{N}(\mathrm{w}; 0, \alpha^{-1} I)$
- **Likelihood**, as before: $p(\mathrm{y}_i/\mathrm{x}_i, \mathrm{w}) = \mathcal{N}(\mathbf{\Phi}_i^T \mathrm{w}, \beta^{-1})$ with $\beta = \frac{1}{2\sigma^2}$
  $\Rightarrow$ **Compute posterior** $p(\mathrm{w}/\mathrm{x}_i, \mathrm{y}_i) \propto p(\mathrm{y}_i/\mathrm{x}_i, \mathrm{w}) p(\mathrm{w})$
  - 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 $p(\mathrm{w}|\alpha) = \mathcal{N}(\mathrm{w}; 0, \alpha^{-1} I)$ and $p(\mathrm{y}_i/\mathrm{x}_i, \mathrm{w}) = \mathcal{N}(\mathbf{\Phi}_i^T \mathrm{w}, \beta^{-1})$, we can show that:

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

- 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]

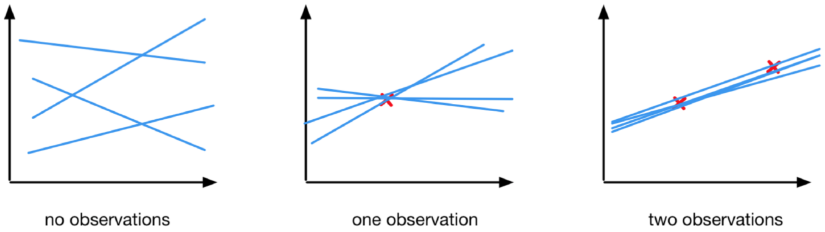
- Assume that:
  - $p(\mathrm{x}) = \mathcal{N}(\mathrm{x}|\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_x)$
  - $p(\mathrm{y}|\mathrm{x}) = \mathcal{N}(\mathrm{y}|A\mathrm{x} + b, \boldsymbol{\Sigma}_y)$
- Then: $p(\mathrm{x}|\mathrm{y}) = \mathcal{N}(\mathrm{x}|\boldsymbol{\mu}_{\mathrm{x}|\mathrm{y}}, \boldsymbol{\Sigma}_{\mathrm{x}|\mathrm{y}})$,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

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

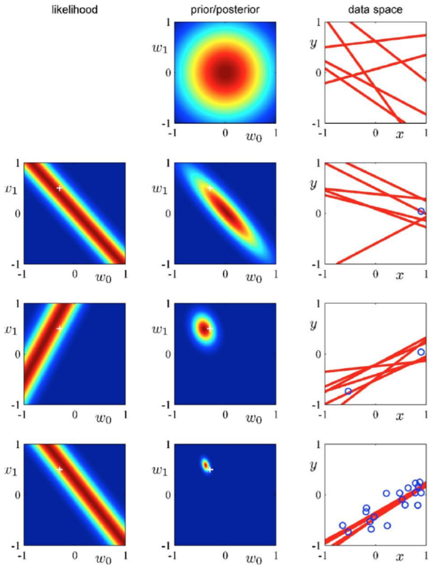
$$\boldsymbol{\mu}_{\mathrm{x}|\mathrm{y}} = \boldsymbol{\Sigma}_{\boldsymbol{x}|\mathrm{y}} \left[\boldsymbol{A}^T \boldsymbol{\Sigma}_y^{-1} (\mathrm{y} - b) + \boldsymbol{\Sigma}_x^{-1} \boldsymbol{\mu}_x \right]$$

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

    ....



Bayesian Linear Regression: Posterior Sampling



0 data points are observed.

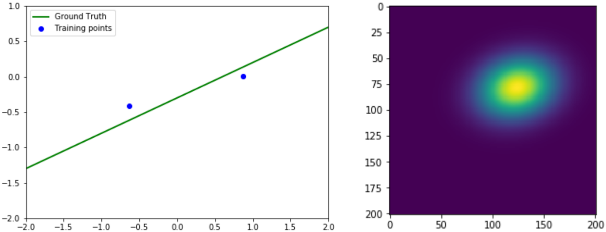
1 data point is observed.

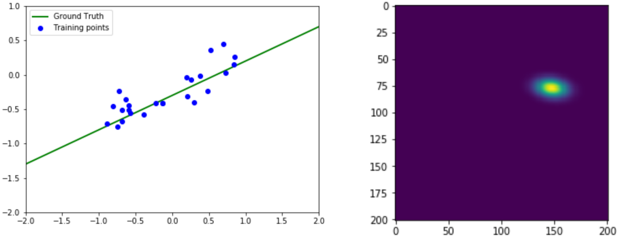
2 data points are observed.

20 data points are observed.

Bayesian Linear Regression: Posterior Sampling

Practical session: compute posterior





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

Bayesian Linear Regression: Predictive Distribution

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

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

Bayesian Linear Regression: Predictive Distribution

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

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

Bayesian Linear Regression: Predictive Distribution

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

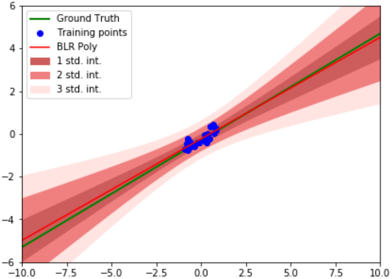
- $\sigma^2_{pred}(\mathrm{x}^*) = \beta^{-1} + \boldsymbol{\Phi}(\mathrm{x}^*)^T \boldsymbol{\Sigma} \boldsymbol{\Phi}(\mathrm{x}^*)$
- $\boldsymbol{\Phi}(\mathrm{x}^*)^T \boldsymbol{\Sigma} \boldsymbol{\Phi}(\mathrm{x}^*)$ is uncertainty over parameters w (**epistemic**)
- **Practical session:** in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

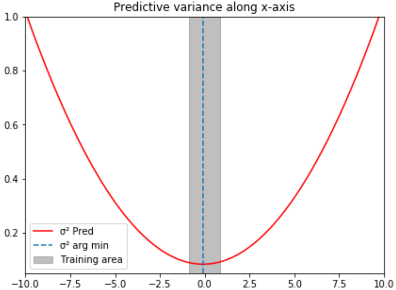
$$\boldsymbol{\Sigma}^{-1} = \alpha \boldsymbol{I} + \beta \boldsymbol{\Phi}^T \boldsymbol{\Phi} = \begin{pmatrix} \alpha + \beta N & \beta 1^T \mathrm{X} \\ \beta 1^T \mathrm{X} & \alpha + \beta \mathrm{X}^T \mathrm{X} \end{pmatrix}$$

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

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

Practical session: predictive distribution and uncertainty





Bayesian Linear Regression

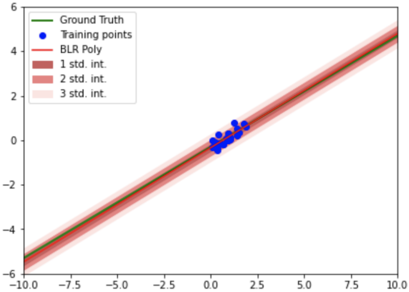
- Note on MAP estimate:

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

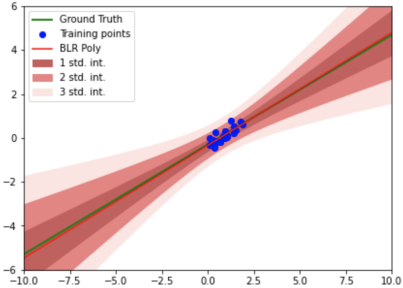
$\Rightarrow$ **adding a Gaussian prior with precision on weights α acts like L_2 regularisation (weight decay) with $\lambda = \alpha/\beta$**

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

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



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

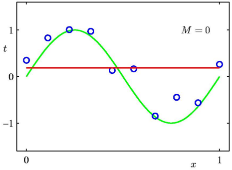


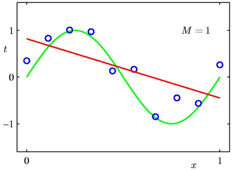
$p(y|\mathrm{x}^*, \mathcal{D}, \alpha, \beta)$

Non-Linear Regression

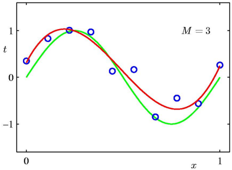
- Linear regression: limited in many datasets
- Non-linear extension by designing explicit non-linear feature maps $\mathbf{\Phi}$
  - Ex: Polynomial regression for 1D input, *i.e.* $x_i \in \mathbb{R}$:

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

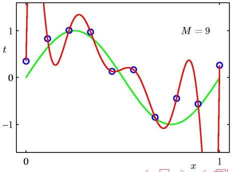




← Poor representations of $\sin(2\pi x)$



← Best Fit to $\sin(2\pi x)$



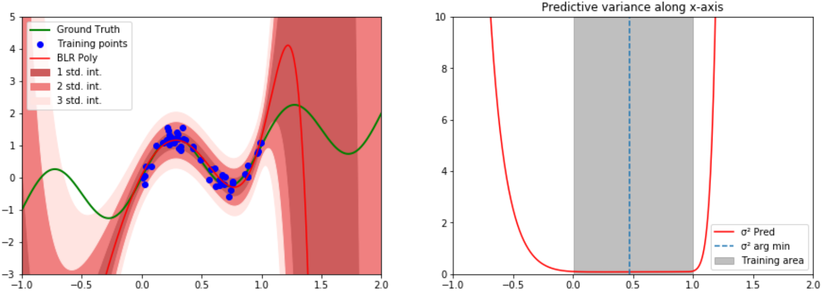
Over Fit Poor representation of $\sin(2\pi x)$

Bayesian Polynomial Regression

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

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

- 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 $f(x) = x + sin(2\Pi x)$, $M = 10$, $\alpha = 0.05$

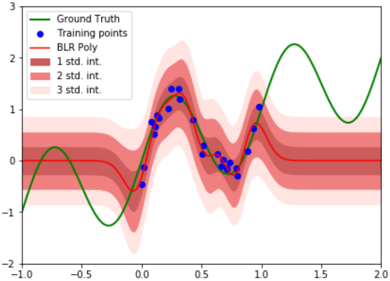


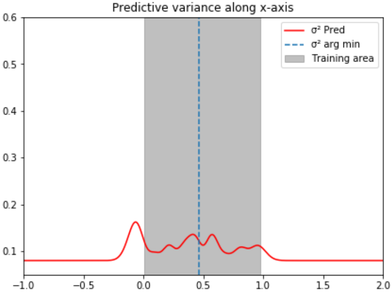
RBF Gaussian Regression

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

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

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





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

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