SF1935 – Probability Theory and Statistics with **Application to Machine Learning**

Lecture 2: Linear models and a probabilistic perspective

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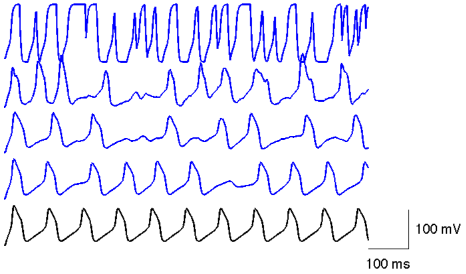
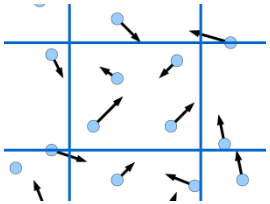
Introduction

Probabilistic approach

- Ubiquitous nature of uncertainty
  - imprecision, noise in data,
  - errors , missing information/data
  - gaps in knowledge, simplified description





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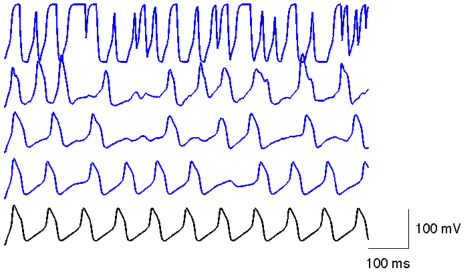

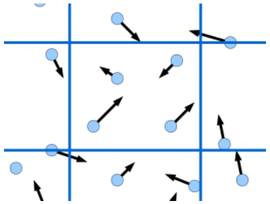

"The theory of probabilities is at bottom nothing but common sense reduced to calculus; it enables us to appreciate with exactness that which accurate minds feel with a sort of instinct for which of times they are unable to account." (Laplace)

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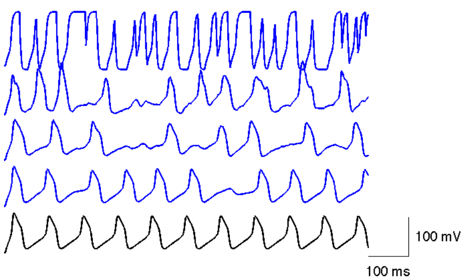
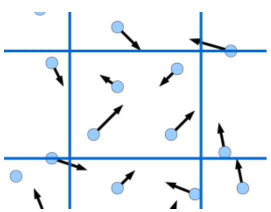


- ➢ Probability theory provides a framework for modelling, reasoning etc. under uncertainty
  - unified, universal, intuitive, interpretable
  - beyond randomness, it is about uncertainty!
  - p. distributions as carriers or information (Jaynes, 2003)



Probabilistic perspective in ML

- Statistical ML: constructing stochastic models
  - fully probabilistic description and inference
  - theoretical assumptions, mathematical tractability, rigour
  - parameters estimated from observed data (learning)
  - interpretability and extra insights
  - machinery to propagate and account for uncertainty effects

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BUT: *can be very hard for large-scale problems* and

difficult to derive solutions in a closed form

Probabilistic perspective in ML

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“ (statistical ML) provides the basis for learning algorithms that directly manipulate probabilities, as well as a framework for analyzing the operation of other algorithms that do not explicitly manipulate probabilities.” Mitchell

Probabilistic perspective in ML

- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)

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  - Apply Bayesian machinery to propagate uncertainty
    - product and sum probability rules, Bayesian theorem

$$p(\mathbf{w} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \mathbf{w})\, p(\mathbf{w})}{p(\mathcal{D})}$$

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

Probabilistic perspective in ML

- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)
  - Apply Bayesian machinery to propagate uncertainty
    - product and sum probability rules, Bayesian theorem
    - the power of marginalisation

$$p(x_1, x_2 .., x_{n-1}) = \int p(x_1, x_2, .., x_n) dx_n$$

$$p(\mathbf{w} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \mathbf{w})\, p(\mathbf{w})}{p(\mathcal{D})}$$

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- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)
  - Apply Bayesian machinery to propagate uncertainty
  - Combine uncertain knowledge with data to reduce uncertainty (based on evidence from observations)
    - batch or sequence where posterior is iteratively updated

Probabilistic perspective in ML

- Philosophy of Bayesian approach
  - Uncertainty is ubiquitous – describe all model components with probabilistic objects (*distributions, not point estimates*)
  - Apply Bayesian machinery to propagate uncertainty
  - Combine uncertain knowledge with data to reduce uncertainty (based on evidence from observations)
  - Two levels of inference:

    parameter estimation and model selection (see Lecture 3)

Back to the probabilistic mindset

Bayesian vs frequentist perspective

I. Probability is a measure of belief (plausibility)

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VI. Probability of the data given hypothesis (likelihood, sampling dist.).

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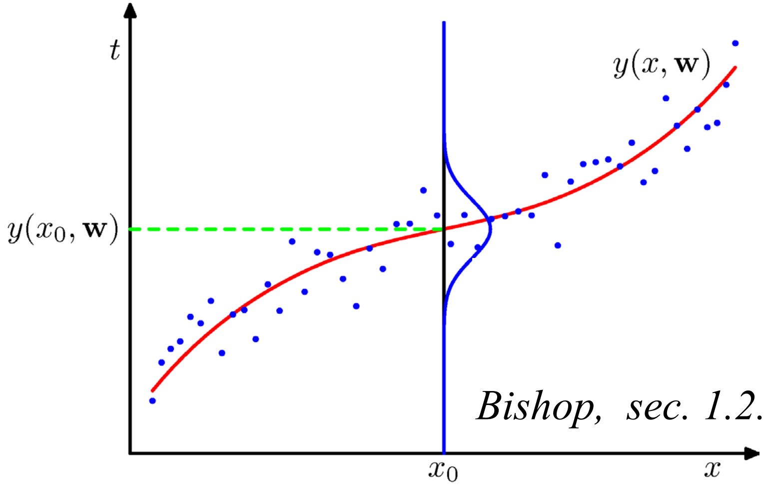
Why isn't everyone Bayesian? *(Efron, 1986)*

Learning as inference

- Learning distributions
  - curve-fitting example: $y(x, \mathbf{w}): X \to Y$ (let's assume polynomial)

$$t = y(x, \mathbf{w}) + \varepsilon$$

observations $\{(x_i, t_i): i=1,..,N\}$: $\mathbf{x} = (x_1, \ldots, x_N)^{\mathrm{T}}$, $\mathbf{t} = (t_1, \ldots, t_N)^{\mathrm{T}}$



Bishop, sec. 1.2.5

Learning as inference

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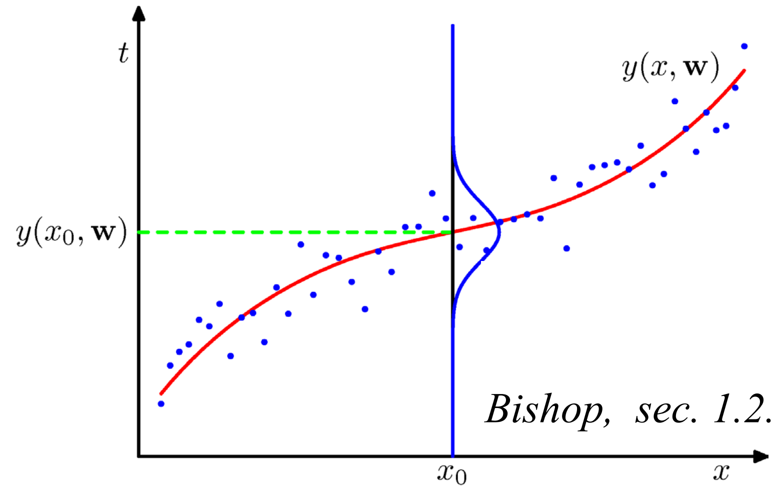
<u>Remarks about notation:</u>

1) here we deal with one-dim input, x and output, t
2) parameters $\boldsymbol{w}$ still constitute a vector (e.g. could be polynomial coefficients)
3) $\mathbf{x}$ and $\mathbf{t}$, refer to the collection of all inputs and outputs, conceptually corresponding to D_x and D_t, but in the vector form, so $\mathbf{x} \rightarrow \mathbf{t}$.



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  - probabilistic framework

$p(\mathbf{w})$ – a prior probability distribution

$p(\mathcal{D} \mid \mathbf{w})$ – the likelihood function for $\mathcal{D} = \mathbf{t}$
(not a probability distrib. over $\mathbf{w}$, just a conditional probability)

$p(\mathbf{w} \mid \mathcal{D})$ – a posterior probability

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Bayes' theorem

$$\color{red}{p(\mathbf{w} \mid \mathcal{D})} = \frac{\color{blue}{p(\mathcal{D} \mid \mathbf{w})}\, \color{green}{p(\mathbf{w})}}{p(\mathcal{D})}$$

$$\color{red}{\text{posterior}} \propto \color{blue}{\text{likelihood}} \times \color{green}{\text{prior}}$$

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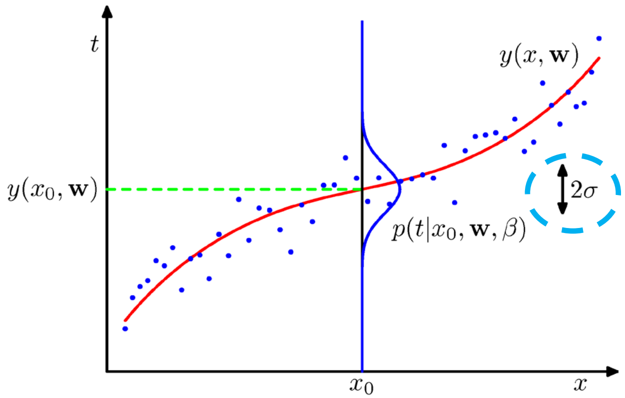
Uncertainty (*noise*) in target data:

$$p(t \mid x, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(x,\mathbf{w}), \beta^{-1})$$

precision



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Learning as inference – estimate parameters

- Learning distributions
  - curve-fitting example: $y(x,\mathbf{w}): X \to Y$ (let's assume polynomial)

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SOLUTION 1

We want to find parameters to be able to use predictive distribution, $p(t|x)$, and infer the target:

$$\mathrm{E}[t \mid x] = \int t\, p(t \mid x, \mathbf{w}_{\mathrm{opt}}, \beta_{\mathrm{opt}})\,\mathrm{d}t$$

Learning as inference – max likelihood

So, we follow the max likelihood approach

ML function for t (i.i.d.) under Gaussian noise $p(t \mid x, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(x, \mathbf{w}), \beta^{-1})$

$$p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n \mid y_n(x_n, \mathbf{w}), \beta^{-1})$$

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The log-likelihood:

$$\boxed{\ln p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)}$$

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Still, input x is one-dim and $\mathbf{x}$ & $\mathbf{t}$ refer to the collection of all data points.

Learning as inference – max likelihood

Maximum likelihood (ML) estimate:

Maximise $$\ln p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi)$$

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$$\mathbf{w}_{\mathrm{ML}} = \arg\min_{\mathbf{w}} \left\{ \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 \right\}$$

the sum-of-squares error function

under the assumption of Gaussian noise : $p(t \mid x, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(x, \mathbf{w}), \beta^{-1})$

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$$\beta_{\mathrm{ML}}^{-1} = \frac{1}{N} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}_{\mathrm{ML}}) - t_n\}^2$$

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$$\boxed{t_{out} = \mathrm{E}[t \mid x_{in}] = \int t \, p(t \mid x_{in}, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) \, \mathrm{d}t}$$

Learning as inference – posterior over parameters

- Learning distributions
  - curve-fitting example: $y(x,\mathbf{w}): X \rightarrow Y$ (let's assume polynomial)

$$t = y(x,\mathbf{w}) + \varepsilon$$

SOLUTION 2

Parameters of the model could also be random variables with a prior distribution, $p(\mathbf{w}\mid\alpha) = \mathcal{N}(\mathbf{w}\mid\mathbf{0},\alpha^{-1}\mathbf{I})$

Now, we must **maximise the posterior** $p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta)$, i.e. find the most probable $\mathbf{w}$ given data:

$$\max\, p(\mathbf{w}\mid\mathbf{x},\mathbf{t},\alpha,\beta) \propto p(\mathbf{t}\mid\mathbf{x},\mathbf{w},\beta)\; p(\mathbf{w}\mid\alpha)$$

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Again, $\boldsymbol{x}$ & $\boldsymbol{t}$ refer to the data collection, not individual input or outputs

Learning as inference – max posterior

Maximum posterior (MAP) estimate:

Maximise $\ln p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta)$

$$\boxed{\mathbf{w}_{\mathrm{MAP}} = \arg\min_{\mathbf{w}} \left\{ \frac{\beta}{2} \sum_{n=1}^{N} \{ y(x_n, \mathbf{w}) - t_n \}^2 + \frac{\alpha}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} \right\}}$$

Learning as inference – recap

Maximum posterior (MAP) estimate:

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BUT: Solutions 1 (ML) and 2 (MAP) give point estimates of $\mathbf{w}$

Learning as inference – Bayesian view

Instead of estimating “optimal” parameters $\mathbf{w}$, let’s integrate over all values of $\mathbf{w}$ (let’s make use of the distribution)

Marginalisation:

$$\underbrace{p(t \mid x, \mathbf{x}, \mathbf{t}, \alpha, \beta)}_{\text{predictive}} = \int \underbrace{p(t \mid x, \mathbf{w}, \beta)}_{\text{“noise” model}} \; \underbrace{p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}, \alpha, \beta)}_{\text{posterior}} \, \mathrm{d}\mathbf{w}$$

We assume we know what α and β are.

Learning as inference – Bayesian view

Instead of estimating "optimal" parameters $\mathbf{w}$, let's integrate over all values of $\mathbf{w}$ for our linear model $y = \sum_{i=0}^{M} w_i \phi_i(x)$

For a one-dim polynomial model: $\phi_i(x) = x^i$ (order M-1)

Learning as inference – Bayesian view

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For a one-dim polynomial model: $\phi_i(x) = x^i$

$$p(t \mid x, \mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}\left(t \mid m(x), s^2(x)\right) \quad \begin{cases} m(x) = \beta\, \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \sum_{n=1}^{N} \boldsymbol{\phi}(x_n)\, t_n \\ s^2(x) = \beta^{-1} + \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S}\, \boldsymbol{\phi}(x) \end{cases}$$

$$\mathbf{S}^{-1} = \alpha \mathbf{I} + \beta \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) \boldsymbol{\phi}(x_n)^{\mathrm{T}}$$

$$\boldsymbol{\phi}(x) = (\phi_0(x), \ldots, \phi_M(x))$$

Learning as inference – summary

In summary:

To use a predictive distribution and infer the output t for the given input x_{in} ....

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To use a predictive distribution and infer the output t for the given input x_{in} ....

.....ML and MAP approaches produce point estimates of $\mathbf{w}$

$$\text{ML}: \quad \mathcal{D} \rightarrow \mathbf{w}_{\text{ML}}$$

$$\text{MAP}: \quad \mathcal{D}, p(\mathbf{w}) \rightarrow \mathbf{w}_{\text{MAP}}$$

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.....in Bayesian approach $\mathbf{w}$ is integrated over (**marginalisation**)

$$\text{Bayes:} \quad \mathcal{D}, p(\mathbf{w}) \to p(\mathbf{w} \mid \mathcal{D})$$

Learning as inference – summary

In summary:

To use a predictive distribution and infer the output t for the given input x_{in} ....

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$$\text{ML}: \quad \mathcal{D} \to \mathbf{w}_{\text{ML}}$$

$$\text{MAP}: \quad \mathcal{D}, p(\mathbf{w}) \to \mathbf{w}_{\text{MAP}}$$

$$\Downarrow$$

Use $p(t \mid x_{in}, \mathbf{w}_{\text{ML}})$ or $p(t \mid x_{in}, \mathbf{w}_{\text{MAP}})$ for prediction.

.....in Bayesian approach $\mathbf{w}$ is integrated over (**marginalisation**)

$$\text{Bayes}: \quad \mathcal{D}, p(\mathbf{w}) \to p(\mathbf{w} \mid \mathcal{D})$$

$$\Downarrow$$

Marginalise over $\mathbf{w}$:

$$p(t \mid \mathcal{D}) = \int p(t \mid x_{in}, \mathbf{w})\, p(\mathbf{w} \mid \mathcal{D})\, \mathrm{d}\mathbf{w}$$

Learning as inference – summary

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$$\text{ML}: \qquad \mathcal{D} \to \mathbf{w}_{\text{ML}}$$

$$\text{MAP}: \qquad \mathcal{D}, p(\mathbf{w}) \to \mathbf{w}_{\text{MAP}}$$

Frequentist philosophy

$p(t \mid x_{in}, \mathbf{w}_{\text{MAP}})$ for prediction.

.....in Bayesian approach $\mathbf{w}$ is integrated over (**marginalisation**)

$$\text{Bayes:} \quad \mathcal{D}, p(\mathbf{w}) \to p(\mathbf{w} \mid \mathcal{D})$$

Bayesian philosophy

$$p(t \mid \mathcal{D}) = \int p(t \mid x_{in}, \mathbf{w})\, p(\mathbf{w} \mid \mathcal{D})\, \mathrm{d}\mathbf{w}$$

Inference and decision (classification)

The ***inference*** stage of classification $\mathcal{D} \rightarrow p(C_k, \boldsymbol{x}), k = 1,..,K$

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starting from *class-conditional* densities and *priors*

Model the inputs $\boldsymbol{x}$ and outputs C

$$\left.\begin{matrix} p(\boldsymbol{x} \mid C_k) \\ p(C_k) \end{matrix}\right\} \text{ for each class } C_k \qquad p(\boldsymbol{x}, C_k)$$

$$p(C_k \mid \boldsymbol{x}) = \frac{p(\boldsymbol{x} \mid C_k)\, p(C_k)}{p(\boldsymbol{x})}$$

$$p(\boldsymbol{x}) = \sum_k p(\boldsymbol{x} \mid C_k)\, p(C_k)$$

GENERATIVE approach

Remarks:
1) K classes
2) $\boldsymbol{x}$ – multi-dim input feature vector

Inference and decision (classification)

The ***inference*** stage of classification $\mathcal{D} \rightarrow p(C_k, \boldsymbol{x}), k = 1,..,K$

Model the inputs $\boldsymbol{x}$ and outputs C

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GENERATIVE approach

Solve first the inference problem of determining ***posteriors*** for each class **without** modelling $p(C_k, \boldsymbol{x})$

$$p(C_k \mid \boldsymbol{x})$$

DISCRIMINATIVE approach

Generative vs discriminative approach

What are the virtues of the generative approach?

- The parameters are estimated separately for each class (no need to retrain the model when new classes are added)
- Rather straightforward to fit in a Bayesian framework (but it depends on the problem, sometimes discriminative function can be easier to optimise)

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  -> generative models can be run "backwards"
- BUT: discriminative models tend to be more accurate (less vulnerable to assumptions)

Bias-variance: frequentist mindset

Expected value over all possible datasets D
(frequentist perspective: data is random)

$$\mathbb{E}[L] = \mathbb{E}_{\mathcal{D}}\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2 + \int \mathrm{var}\left[t \mid \boldsymbol{x}\right] p(\boldsymbol{x})\, d\boldsymbol{x}$$

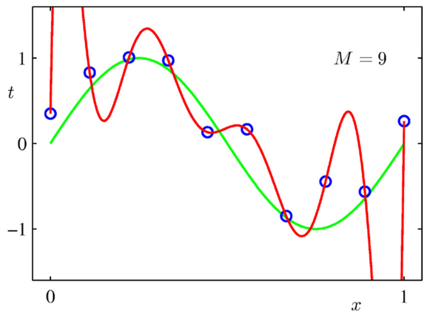
$$\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2 = \left\{y(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] + \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] - h(\boldsymbol{x})\right\}^2$$

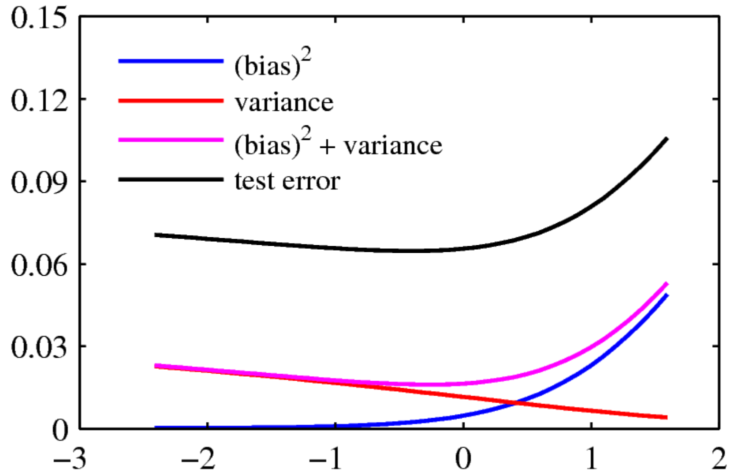
$$\mathbb{E}_{\mathcal{D}}\left[\left\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\right\}^2\right] = \underbrace{\left\{\mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right] - h(\boldsymbol{x})\right\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left\{y(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\boldsymbol{x};\mathcal{D})\right]\right\}^2\right]}_{\text{variance}}$$

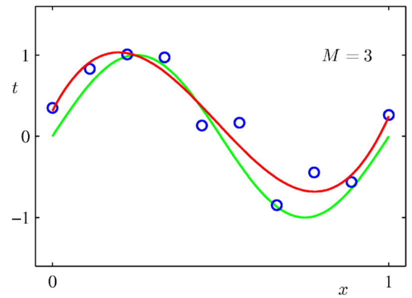
Bias-variance as a frequentist dilemma

$$\mathbb{E}_{\mathcal{D}}[L] = \mathbb{E}_{\mathcal{D}}\{y(\boldsymbol{x};\mathcal{D}) - h(\boldsymbol{x})\}^2 + \int \mathrm{var}[t\,|\,\boldsymbol{x}]\,p(\boldsymbol{x})\,dx$$

$$\mathbb{E}[L] = (\text{bias})^2 + \text{variance} + \text{noise}$$







increased model complexity

Bishop, sec. 3.2

Model selection: frequentist vs Bayesian

- Occam's razor – *"Accept the simplest explanation that fits the data."*
- Frequentist approach with maximum likelihood
  - bias-variance dilemma
  - need to control the model's complexity
    - regularisation
    - correction for the bias of ML estimates (AIC, BIC)
    - empirical estimate of generalisation error on a hold-out set (validation, resampling)
    - structural risk minimization (SRM) (minimise upper bound on the true risk), see also VC dimension (statistical learning theory)

Model selection: frequentist vs Bayesian

- Occam's razor – *"Accept the simplest explanation that fits the data."*
- Frequentist approach with maximum likelihood
- Bayesian approach using model evidence

$$p(\mathbf{w} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \mathbf{w})\, p(\mathbf{w})}{p(\mathcal{D})} \Longrightarrow p(\mathbf{w} \mid \mathcal{D}, \mathcal{M}_i) = \frac{p(\mathcal{D} \mid \mathbf{w}, \mathcal{M}_i)\, p(\mathbf{w} \mid \mathcal{M}_i)}{p(\mathcal{D} \mid \mathcal{M}_i)}$$

$p(\mathcal{D})$ shows where the model spreads its probability mass over the data space

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$p(\mathcal{D})$ shows where the model spreads its probability mass over the data space

Towards the posterior: $p(\mathcal{M}_i \mid \mathcal{D}) \propto p(\mathcal{M}_i)\, p(\mathcal{D} \mid \mathcal{M}_i)$

marginal likelihood

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calculating $p(\mathcal{D} \mid \mathcal{M}_i)$ is not so trivial:

$$p(\mathcal{D} \mid \mathcal{M}_i) = \int p(\mathcal{D} \mid \mathbf{w}, \mathcal{M}_i)\, p(\mathbf{w} \mid \mathcal{M}_i)\, d\mathbf{w}$$

"The evidence can be seen as the probability of generating the data set from a model whose parameters are sampled at random from the prior"