Advanced Machine Learning
Summer 2019

Part 2 – Linear Regression
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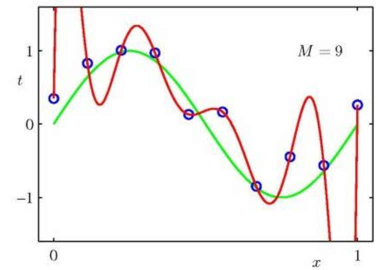
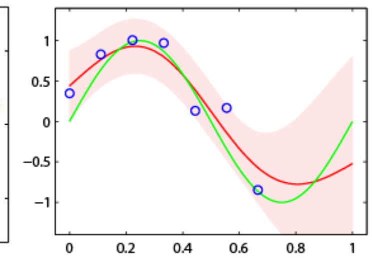
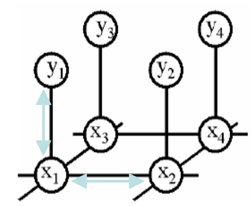
Course Outline

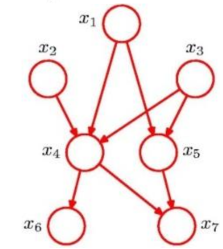
- Regression Techniques
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Bayesian Regression
- Deep Reinforcement Learning
- Probabilistic Graphical Models
  - Bayesian Networks
  - Markov Random Fields
  - Inference (exact & approximate)
- Deep Generative Models
  - Generative Adversarial Networks
  - Variational Autoencoders

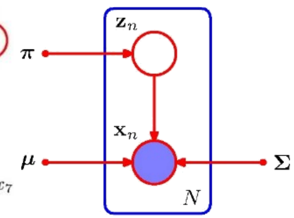
$$f : \mathcal{X} \rightarrow \mathbb{R}$$

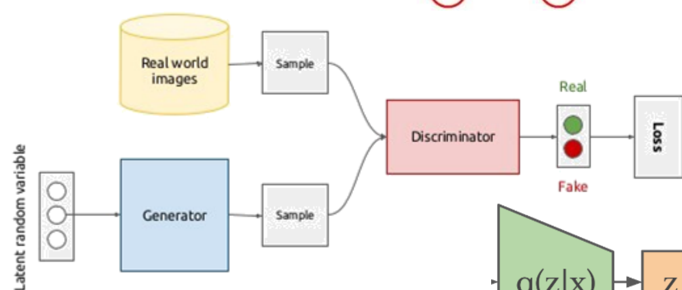


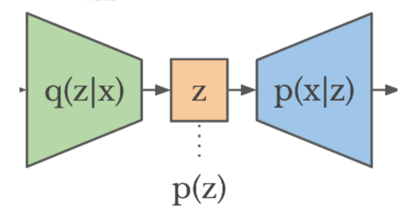












Topics of This Lecture

- Recap: Important Concepts from ML Lecture
  - Probability Theory
  - Bayes Decision Theory
  - Maximum Likelihood Estimation
  - *New:* Bayesian Estimation
- A Probabilistic View on Regression
  - Least-Squares Estimation as Maximum Likelihood
  - Predictive Distribution
  - Maximum-A-Posteriori (MAP) Estimation
  - Bayesian Curve Fitting
- Discussion

Recap: The Rules of Probability

- Basic rules

Sum Rule $$p(X) = \sum_Y p(X, Y)$$

Product Rule $$p(X, Y) = p(Y|X)p(X)$$

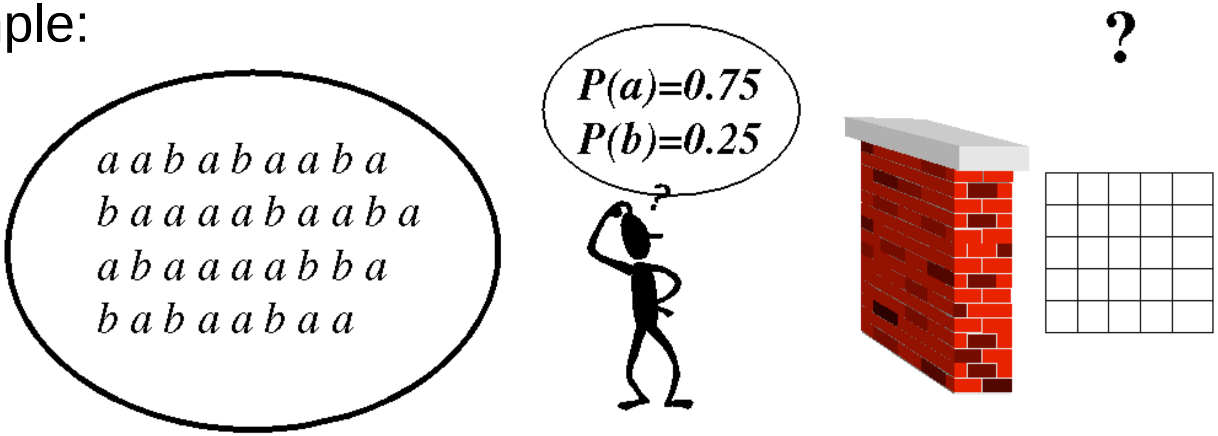
- From those, we can derive

Bayes' Theorem $$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

where $$p(X) = \sum_Y p(X|Y)p(Y)$$

Recap: Bayes Decision Theory

- Concept 1: Priors (a priori probabilities) $\boxed{p(C_k)}$
  - What we can tell about the probability *before seeing the data*.
  - Example:



$$C_1 = a \qquad p(C_1) = 0.75$$

$$C_2 = b \qquad p(C_2) = 0.25$$

- In general: $\sum_k p(C_k) = 1$

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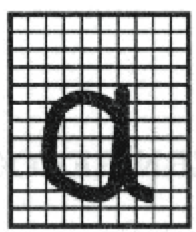
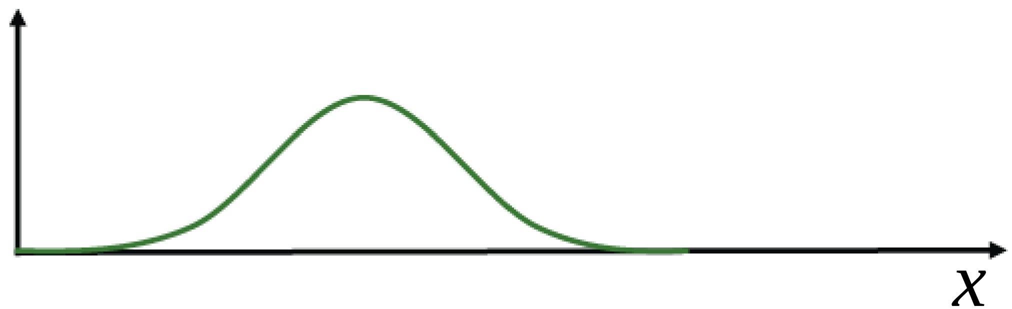
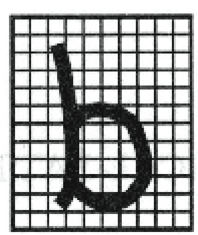
Recap: Bayes Decision Theory

- Concept 2: Conditional probabilities $\boxed{p(x|C_k)}$
  - Let x be a feature vector.
  - x measures/describes certain properties of the input.
    - E.g. number of black pixels, aspect ratio, …
  - $p(x|C_k)$ describes its likelihood for class C_k.

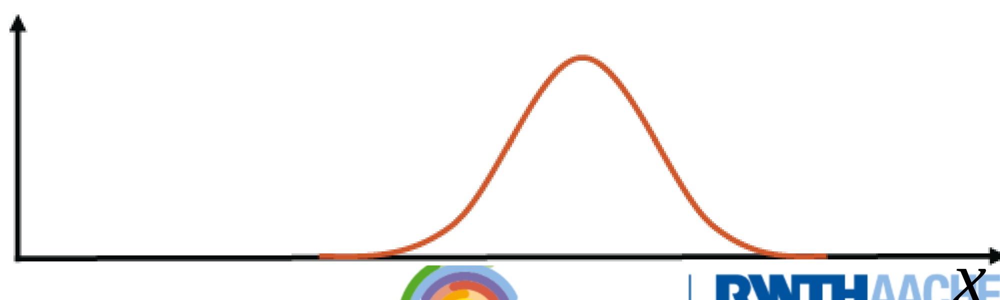


$p(x|a)$





$p(x|b)$



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Recap: Bayes Decision Theory

- Concept 3: Posterior probabilities $\boxed{p(C_k \mid x)}$
  - We are typically interested in the *a posteriori* probability, i.e. the probability of class C_k given the measurement vector x.
- Bayes' Theorem:

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

- Interpretation

$$Posterior = \frac{Likelihood \times Prior}{Normalization\ Factor}$$

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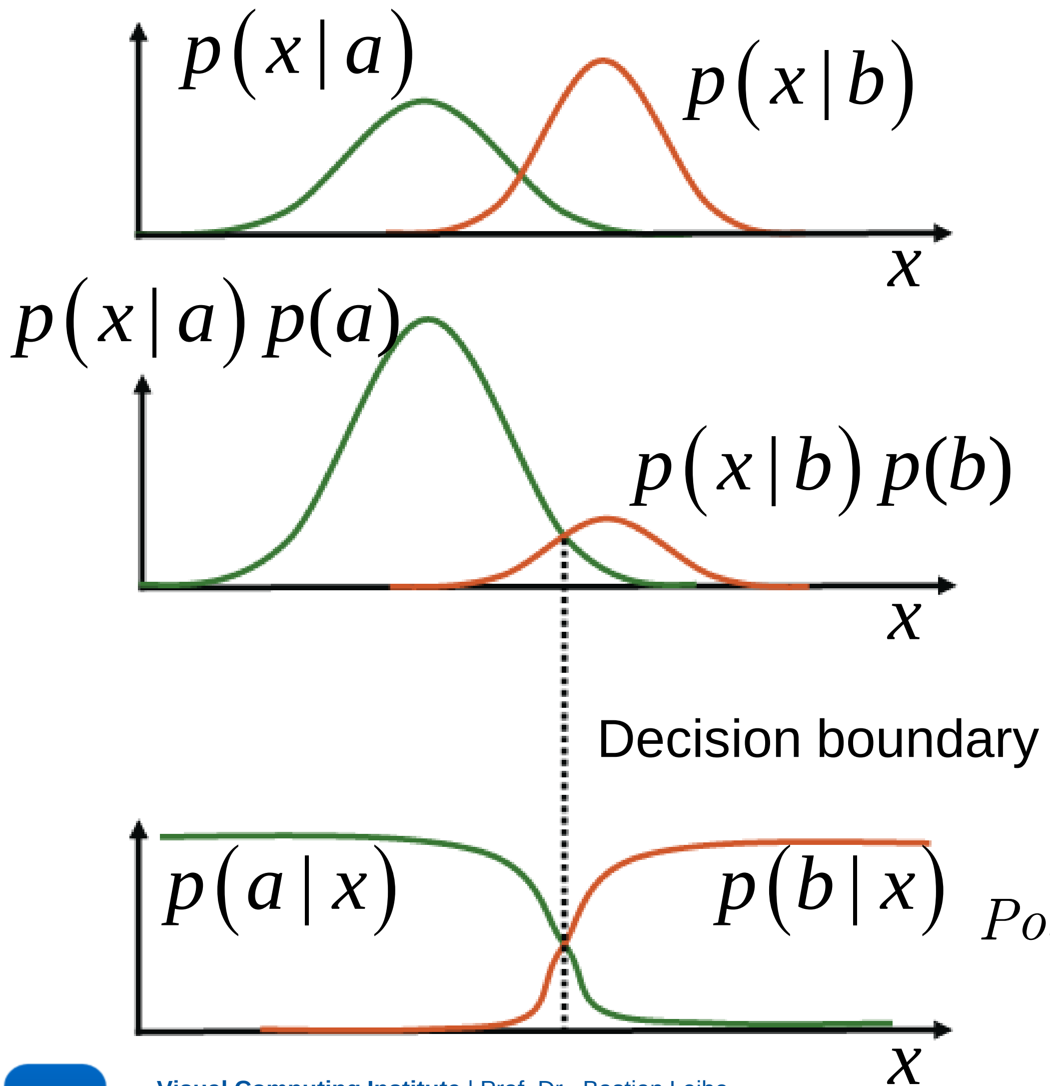
Recap: Bayes Decision Theory



$$Likelihood$$

$$Likelihood \times Prior$$

$$Posterior = \frac{Likelihood \times Prior}{NormalizationFactor}$$

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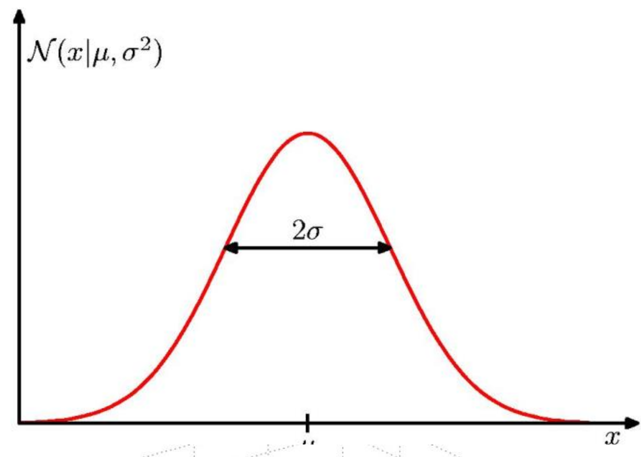
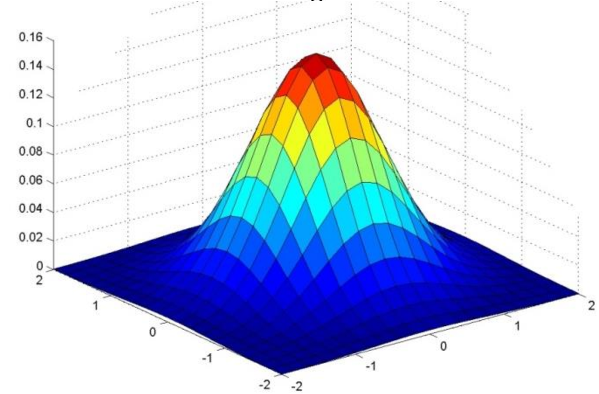
Recap: Gaussian (or Normal) Distribution

- One-dimensional case
  - Mean μ
  - Variance σ^2



$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

- Multi-dimensional case
  - Mean μ
  - Covariance Σ

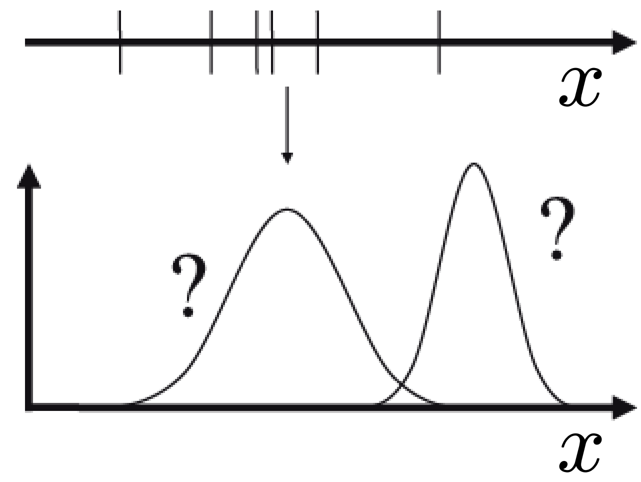


$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Image source: C.M. Bishop, 2006

Recap: Parametric Methods for Prob. Density Estimation

- Given
  - Data $X = \{x_1, x_2, \ldots, x_N\}$
  - Parametric form of the distribution with parameters θ
  - E.g. for Gaussian distrib.: $\theta = (\mu, \sigma)$



- Learning
  - Estimation of the parameters θ

- Likelihood of θ
  - Probability that the data X have indeed been generated from a probability density with parameters θ

$$L(\theta) = p(X|\theta)$$

Slide adapted from Bernt Schiele

Recap: Maximum Likelihood Approach

- Computation of the likelihood
  - Single data point: $p(x_n|\theta) = \mathcal{N}(x_n|\mu, \sigma^2)$
  - Assumption: all data points $X = \{x_1, \ldots, x_n\}$ are independent

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

  - Log-likelihood

$$E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$$

- Learning = Estimation of the parameters θ
  - Maximize the likelihood (=minimize the negative log-likelihood)

$\Rightarrow$ Take the derivative and set it to zero.

$$\frac{\partial}{\partial\theta} E(\theta) = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial\theta} p(x_n|\theta)}{p(x_n|\theta)} \stackrel{!}{=} 0$$

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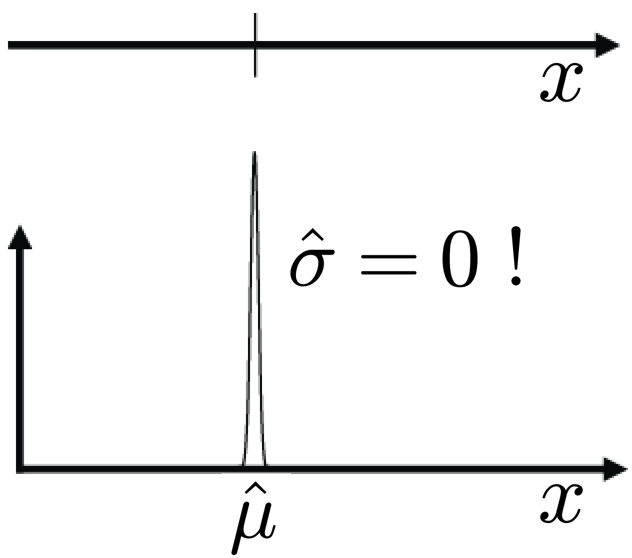
Recap: Maximum Likelihood Approach

- Maximum Likelihood has several significant limitations
  - It systematically underestimates the variance of the distribution!
  - E.g. consider the case

$$N = 1, X = \{x_1\}$$



$\Rightarrow$ Maximum-likelihood estimate:

  - We say ML *overfits to the observed data*.
  - We will still often use ML, but it is important to know about this effect.

Slide adapted from Bernt Schiele

Deeper Reason

- Maximum Likelihood is a Frequentist concept
  - In the Frequentist view, probabilities are the *frequencies of random, repeatable events*.
  - These frequencies are fixed, but can be estimated more precisely when more data is available.
- This is in contrast to the Bayesian interpretation
  - In the Bayesian view, probabilities quantify the *uncertainty about certain states or events*.
  - This uncertainty can be revised in the light of new evidence.
- Bayesians and Frequentists do not like each other too well…

Bayesian vs. Frequentist View

- To see the difference…
  - Suppose we want to estimate the uncertainty whether the Arctic ice cap will have disappeared by the end of the century.
  - This question makes no sense in a Frequentist view, since the event cannot be repeated numerous times.
  - In the Bayesian view, we generally have a prior, e.g. from calculations how fast the polar ice is melting.
  - If we now get fresh evidence, e.g. from a new satellite, we may revise our opinion and update the uncertainty from the prior.

$$Posterior \propto Likelihood \times Prior$$

  - This generally allows to get better uncertainty estimates for many situations.
- Main Frequentist criticism
  - The prior has to come from somewhere and if it is wrong, the result will be worse.

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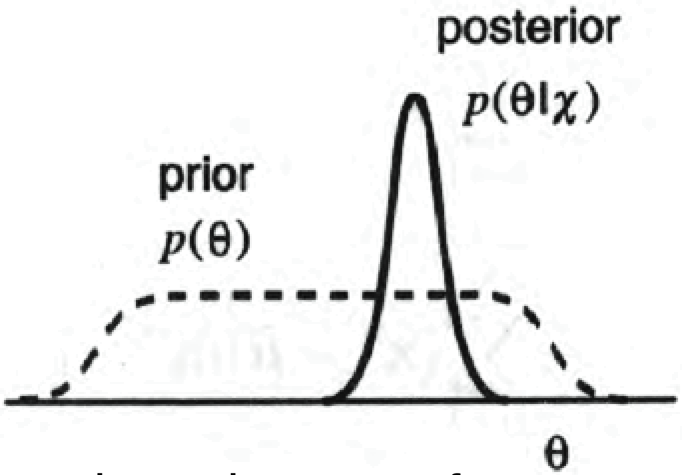
Bayesian Approach to Parameter Learning

- Conceptual shift
  - Maximum Likelihood views the true parameter vector θ to be unknown, but fixed.
  - In Bayesian learning, we consider θ to be a random variable.
- This allows us to use knowledge about the parameters θ
  - i.e., to use a prior for θ
  - Training data then converts this prior distribution on θ into a posterior probability density.



  - The prior thus encodes knowledge we have about the type of distribution we expect to see for θ.

Slide adapted from Bernt Schiele

Bayesian Learning Approach

- Bayesian view:
  - Consider the parameter vector θ as a random variable.
  - When estimating the parameters, what we compute is

$$p(x|X) = \int p(x, \theta|X) d\theta$$

$$p(x, \theta|X) = p(x|\theta, \cancel{X}) p(\theta|X)$$

Assumption: given θ, this doesn't depend on X anymore

$$p(x|X) = \int \underbrace{p(x|\theta)} p(\theta|X) d\theta$$

This is entirely determined by the parameter θ (i.e., by the parametric form of the pdf).

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Bayesian Learning Approach

$$p(x|X) = \int p(x|\theta)\underbrace{p(\theta|X)}d\theta$$

$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)} = \frac{p(\theta)}{\underbrace{p(X)}}L(\theta)$$

$$p(X) = \int p(X|\theta)p(\theta)d\theta = \int L(\theta)p(\theta)d\theta$$

– Inserting this above, we obtain

$$p(x|X) = \int \frac{p(x|\theta)L(\theta)p(\theta)}{p(X)}d\theta = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\int L(\theta)p(\theta)d\theta}d\theta$$

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Bayesian Learning Approach

- Discussion

Likelihood of the parametric form θ given the data set X.

Estimate for x based on parametric form θ

Prior for the parameters θ

$$p(x|X) = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\underbrace{\int L(\theta)p(\theta)d\theta}}d\theta$$

Normalization: integrate over all possible values of θ

$\Rightarrow$ *The parameter values θ are not the goal, just a means to an end.*

Bayesian Learning Approach

- Discussion

$$p(x|X) = \int p(x|\theta)p(\theta|X)d\theta = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\int L(\theta)p(\theta)d\theta}d\theta$$

  - The probability $p(\theta|X)$ makes the dependency of the estimate on the data explicit.
  - If $p(\theta|X)$ is very small everywhere, but is large for one $\hat{\theta}$, then

$$p(x|X) \approx p(x|\hat{\theta})$$

  $\Rightarrow$ The more uncertain we are about θ, the more we average over all parameter values.

- Problem
  - In the general case, exact integration over θ is not possible / feasible.

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Curve Fitting Revisited

- We've looked at curve fitting in terms of error minimization…
- Now view the problem from a probabilistic perspective
  - Goal is to make predictions for target variable t given new value for input variable x.
  - Basis: training set $\mathbf{x} = (x_1, \ldots, x_N)^{\mathrm{T}}$ with target values $\mathbf{t} = (t_1, \ldots, t_N)^{\mathrm{T}}$.
  - We express our uncertainty over the value of the target variable using a probability distribution

$$p(t|x, \mathbf{w}, \beta)$$

Probabilistic Regression

- First assumption:
  - Our target function values y are generated by adding noise to the function estimate:

$$y = f(\mathbf{x}, \mathbf{w}) + \epsilon$$

Target function value

Noise

Regression function (previously $y(\cdot)$)

Input value

Weights or parameters

- Second assumption:
  - The noise is Gaussian distributed

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

Mean

Variance (β precision)

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Assumption: Gaussian Noise

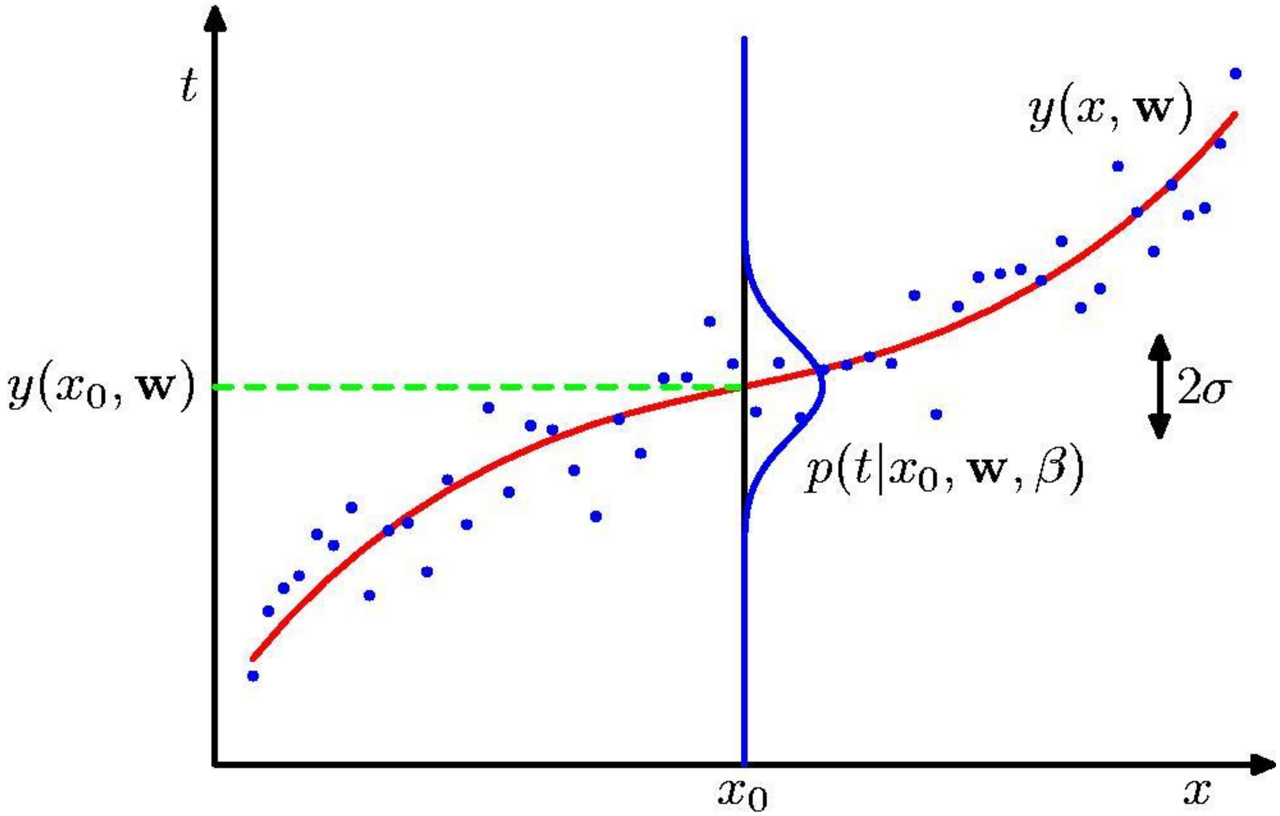

Image source: C.M. Bishop, 2006

Probabilistic Regression

- Given
  - Training data points: $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
  - Associated function values: $\mathbf{y} = [y_1, \ldots, y_n]^T$

- Conditional likelihood (assuming i.i.d. data)

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{i=1}^{n} \mathcal{N}(y_i | f(\mathbf{x}_i, \mathbf{w}), \beta^{-1}) = \prod_{i=1}^{n} \mathcal{N}(y_i | \underbrace{\mathbf{w}^T \phi(\mathbf{x}_i)}, \beta^{-1})$$

$\Rightarrow$ Maximize w.r.t. $\mathbf{w}$, β

Generalized linear regression function

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Maximum Likelihood Regression

- Simplify the log-likelihood

$$
\begin{aligned}
\log p(\mathbf{y}|\mathbf{X},\mathbf{w},\beta) &= \sum_{i=1}^{n} \log \mathcal{N}(y_i|\mathbf{w}^T\phi(\mathbf{x}_i),\beta^{-1}) \\
&= \sum_{i=1}^{n} \left[\log\left(\frac{\sqrt{\beta}}{\sqrt{2\pi}}\right) - \frac{\beta}{2}(y_i - \mathbf{w}^T\phi(\mathbf{x}_i))^2\right] \\
&= \frac{n}{2}\log\beta - \frac{n}{2}\log(2\pi) - \frac{\beta}{2}\sum_{i=1}^{n}(y_i - \mathbf{w}^T\phi(\mathbf{x}_i))^2
\end{aligned}
$$

- Gradient w.r.t. $\mathbf{w}$:

$$
\nabla_{\mathbf{w}} \log p(\mathbf{y}|\mathbf{X},\mathbf{w},\beta) = -\beta\sum_{i=1}^{n}(y_i - \mathbf{w}^T\phi(\mathbf{x}_i))\phi(\mathbf{x}_i)
$$

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Maximum Likelihood Regression

$$\nabla_{\mathbf{w}} \log p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \beta) \;=\; -\beta \sum_{i=1}^{n} (y_i - \mathbf{w}^T \phi(\mathbf{x}_i))\phi(\mathbf{x}_i)$$

- Setting the gradient to zero:

$$0 \;=\; -\beta \sum_{i=1}^{n} (y_i - \mathbf{w}^T \phi(\mathbf{x}_i))\phi(\mathbf{x}_i)$$

$$\Leftrightarrow \quad \sum_{i=1}^{n} y_i \phi(\mathbf{x}_i) = \left[\sum_{i=1}^{n} \phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^T \right] \mathbf{w}$$

$$\Leftrightarrow \quad \mathbf{\Phi y} = \mathbf{\Phi \Phi}^T \mathbf{w} \qquad\qquad \mathbf{\Phi} = [\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)]$$

$$\Leftrightarrow \quad \mathbf{w}_{\mathrm{ML}} = (\mathbf{\Phi \Phi}^T)^{-1} \mathbf{\Phi y}$$

Same as in least-squares regression!

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Maximum Likelihood Regression

$$\nabla_{\mathbf{w}} \log p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \beta) \;=\; -\beta \sum_{i=1}^{n} (y_i - \mathbf{w}^T \phi(\mathbf{x}_i))\phi(\mathbf{x}_i)$$

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$$\Leftrightarrow \quad \mathbf{w}_{\mathrm{ML}} = (\mathbf{\Phi \Phi}^T)^{-1} \mathbf{\Phi y}$$

$\Rightarrow$ *Least-squares regression is equivalent to Maximum Likelihood under the assumption of Gaussian noise.*

Slide credit: Bernt Schiele

Role of the Precision Parameter

- Also use ML to determine the precision parameter β:

$$\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \frac{N}{2}\log\beta - \frac{N}{2}\log(2\pi)$$

- Gradient w.r.t. β:

$$\nabla_\beta \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = -\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \frac{N}{2}\frac{1}{\beta}$$

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2$$

$\Rightarrow$ *The inverse of the noise precision is given by the residual variance of the target values around the regression function.*

Predictive Distribution

- Having determined the parameters $\mathbf{w}$ and β, we can now make predictions for new values of $\mathbf{x}$.

$$p(t|\mathbf{X}, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1})$$

- This means
  - Rather than giving a point estimate, we can now also give an estimate of the estimation uncertainty.

- *What else can we do in the Bayesian view of regression?*

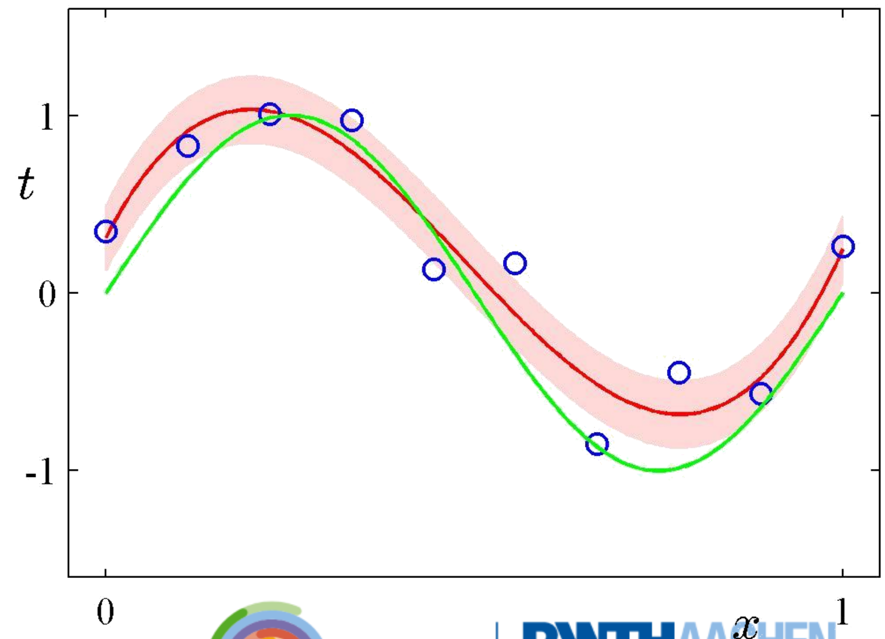

Image source: C.M. Bishop, 2006

MAP: A Step Towards Bayesian Estimation…

- Introduce a prior distribution over the coefficients $\mathbf{w}$.
  - For simplicity, assume a zero-mean Gaussian distribution

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right\}$$

  - New hyperparameter α controls the distribution of model parameters.

- Express the posterior distribution over $\mathbf{w}$.
  - Using Bayes' theorem:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \beta, \alpha) \propto p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

  - We can now determine $\mathbf{w}$ by maximizing the posterior.
  - This technique is called maximum-a-posteriori (MAP).

MAP Solution

- Minimize the negative logarithm

$$-\log p(\mathbf{w}|\mathbf{X},\mathbf{t},\beta,\alpha) \propto -\log p(\mathbf{t}|\mathbf{X},\mathbf{w},\beta) - \log p(\mathbf{w}|\alpha)$$

$$-\log p(\mathbf{t}|\mathbf{X},\mathbf{w},\beta) = \frac{\beta}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n,\mathbf{w}) - t_n\}^2 + \text{const}$$

$$-\log p(\mathbf{w}|\alpha) = \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \text{const}$$

- The MAP solution is therefore the solution of

$$\frac{\beta}{2}\sum_{n=1}^{N}\{y(\mathbf{x}_n,\mathbf{w}) - t_n\}^2 + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w}$$

$\Rightarrow$ *Maximizing the posterior distribution is equivalent to minimizing the regularized sum-of-squares error (with* $\lambda = \frac{\alpha}{\beta}$*).*

Results of Probabilistic View on Regression

- Better understanding what linear regression *means:*
  - *Least-squares regression is equivalent to ML estimation under the assumption of Gaussian noise*.

  $\Rightarrow$ We can use the predictive distribution to give an uncertainty estimate on the prediction.

  $\Rightarrow$ But: known problem with ML that it tends towards overfitting.

  - *L2-regularized regression (Ridge regression) is equivalent to MAP estimation with a Gaussian prior on the parameters* $\mathbf{w}$.

  $\Rightarrow$ The prior controls the parameter values to reduce overfitting.

  $\Rightarrow$ This gives us a tool to explore more general priors.

- But still no full Bayesian Estimation yet
  - Should integrate over all values of $\mathbf{w}$ instead of just making a point estimate.

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Bayesian Curve Fitting

- Given
  - Training data points: $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
  - Associated function values: $\mathbf{t} = [t_1, \ldots, t_n]^T$
  - Our goal is to predict the value of t for a new point $\mathbf{x}$.

- Evaluate the predictive distribution

$$p(t|x, \mathbf{X}, \mathbf{t}) = \int \underbrace{p(t|x, \mathbf{w})} \underbrace{p(\mathbf{w}|\mathbf{X}, \mathbf{t})} d\mathbf{w}$$

What we just computed for MAP

  - Noise distribution – again assume a Gaussian here

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

  - Assume that parameters α and β are fixed and known for now.

Bayesian Curve Fitting

- Under those assumptions, the posterior distribution is a Gaussian and can be evaluated analytically:

$$p(t|x, \mathbf{X}, \mathbf{t}) = \mathcal{N}(t|m(x), s^2(x))$$

  – where the mean and variance are given by

$$m(x) = \beta\phi(x)^T \mathbf{S} \sum_{n=1}^{N} \phi(\mathbf{x}_n) t_n$$

$$s(x)^2 = \beta^{-1} + \phi(x)^T \mathbf{S} \phi(x)$$

  – and $\mathbf{S}$ is the regularized covariance matrix

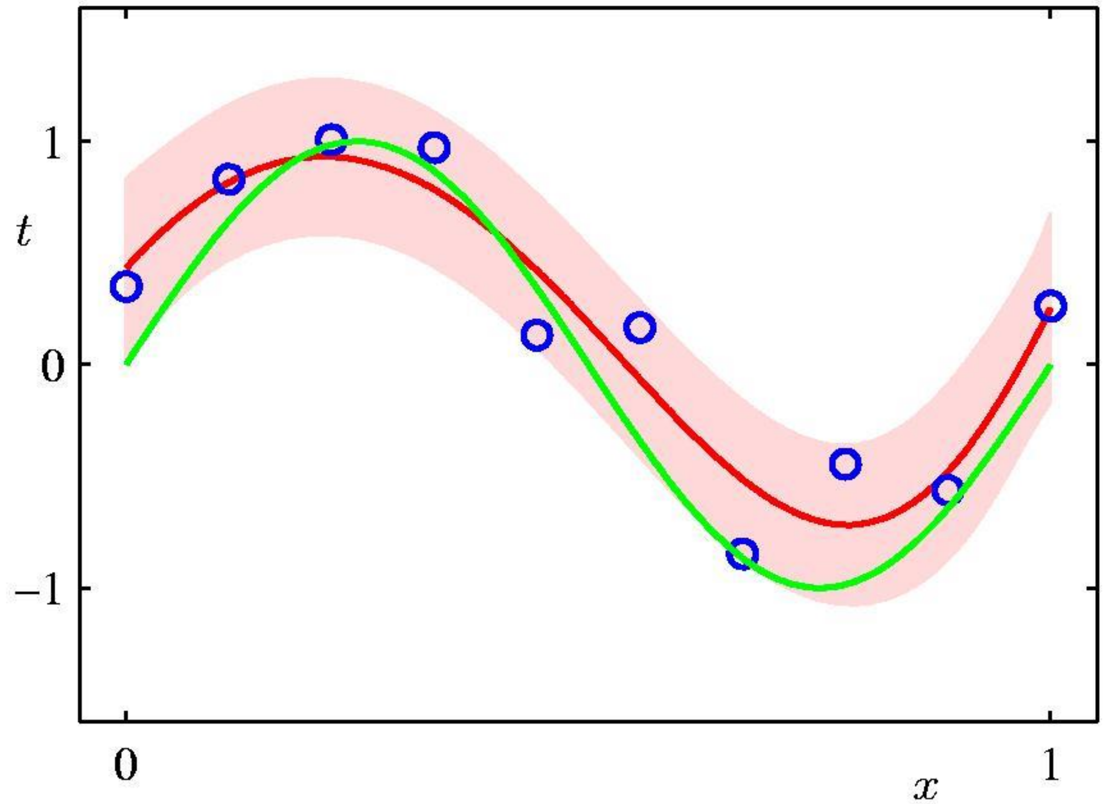
$$\mathbf{S}^{-1} = \alpha\mathbf{I} + \beta \sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^T$$

Analyzing the result

- Analyzing the variance of the predictive distribution

$$s(x)^2 = \underbrace{\beta^{-1}}_{\text{Uncertainty in the predicted value due to noise on the target variables (expressed already in ML)}} + \underbrace{\phi(x)^T \mathbf{S} \phi(x)}_{\text{Uncertainty in the parameters } \mathbf{w} \text{ (consequence of Bayesian treatment)}}$$

Bayesian Predictive Distribution



- Important difference to previous example
  - Uncertainty may vary with test point x!

$$s(x)^2 = \beta^{-1} + \phi(x)^T \mathbf{S} \phi(x)$$

Image source: C.M. Bishop, 2006

Topics of This Lecture

- Recap: Important Concepts from ML Lecture
  - Probability Theory
  - Bayes Decision Theory
  - Maximum Likelihood Estimation
  - Bayesian Estimation
- A Probabilistic View on Regression
  - Least-Squares Estimation as Maximum Likelihood
  - Predictive Distribution
  - Maximum-A-Posteriori (MAP) Estimation
  - Bayesian Curve Fitting
- Discussion

Discussion

- We now have a better understanding of regression.
  - Least-squares regression: Assumption of Gaussian noise

  $\Rightarrow$ We can now also plug in different noise models and explore how they affect the error function.

  - L2 regularization as a Gaussian prior on parameters $\mathbf{w}$.

  $\Rightarrow$ We can now also use different regularizers and explore what they mean.

  $\Rightarrow$ Next lecture…

  - General formulation with basis functions $\phi(\mathbf{x})$.

  $\Rightarrow$ We can now also use different basis functions.

Discussion (2)

- General regression formulation
  - In principle, we can perform regression in arbitrary spaces and with many different types of basis functions
  - However, there is a caveat… Can you see what it is?

- Example: Polynomial curve fitting, $M = 3$

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{i=1}^{D} w_i x_i + \sum_{i=1}^{D} \sum_{j=1}^{D} w_{ij} x_i x_j + \sum_{i=1}^{D} \sum_{j=1}^{D} \sum_{k=1}^{D} w_{ijk} x_i x_j x_k$$

$\Rightarrow$ Number of coefficients grows with D^M!

$\Rightarrow$ The approach becomes quickly unpractical for high dimensions.

  - This is known as the curse of dimensionality.
  - We will encounter some ways to deal with this later.

References and Further Reading

- More information on linear regression can be found in Chapters 1.2.5-1.2.6 and 3.1-3.1.4 of

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006