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## 3. Regression

#### **Categories of Learning (Rep.)**









### Mathematical Formulation (Rep.)

Suppose we are given a set  $\mathcal{X}$  of objects and a set  $\mathcal{Y}$  of object categories (classes). In the learning task we search for a mapping  $\varphi : \mathcal{X} \to \mathcal{Y}$  such that *similar* elements in  $\mathcal{X}$  are mapped to *similar* elements in  $\mathcal{Y}$ .

#### Difference between regression and classification:

- In regression,  ${\mathcal Y}$  is  ${\it continuous},$  in classification it is discrete
- Regression learns a function, classification usually learns class labels

#### For now we will treat regression



#### **Basis Functions**

In principal, the elements of  $\mathcal{X}$  can be anything (e.g. real numbers, graphs, 3D objects). To be able to treat these objects mathematically we need functions  $\phi$  that map from  $\mathcal{X}$  to  $\mathbb{R}^N$ . We call these the **basis functions**.

We can also interpret the basis functions as functions that extract features from the input data.

Features reflect the properties of the objects (width, height, etc.).





#### Simple Example: Linear Regression

- Assume:  $\mathcal{X} = \mathbb{R}, \ \mathcal{Y} = \mathbb{R}, \ \phi = I$  (identity)
- Given: data points  $(x_1, t_1), (x_2, t_2), \dots$
- **Goal:** predict the value *t* of a new example *x*
- Parametric formulation:  $y(x, \mathbf{w}) = w_0 + w_1 x$





#### **Linear Regression**

To evaluate the function *y*, we need an error function:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} (y(x_i, \mathbf{w}) - t_i)^2$$
 "Sum of  
Squared Errors"

We search for parameters  $\mathbf{w}^*$  s.th.  $E(\mathbf{w}^*)$  is minimal:

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{\infty} (y(x_i, \mathbf{w}) - t_i) \nabla y(x_i, \mathbf{w}) \doteq (0 \quad 0)$$

$$y(x_i, \mathbf{w}) = w_0 + w_1 x_i \qquad \Rightarrow \qquad \nabla y(x_i, \mathbf{w}) = (1 \quad x_i)$$

Using vector notation:  $\mathbf{x}_i := (1 \quad x_i)^T \qquad y(x_i, \mathbf{w}) = \mathbf{w}^T \mathbf{x}_i$ 

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{N} \mathbf{w}^{T} \mathbf{x}_{i} \mathbf{x}_{i}^{T} - \sum_{i=1}^{N} t_{i} \mathbf{x}_{i}^{T} = (0 \quad 0) \Rightarrow \mathbf{w}^{T} \sum_{\substack{i=1\\ =:A^{T}}}^{N} \mathbf{x}_{i} \mathbf{x}_{i}^{T} = \sum_{\substack{i=1\\ =:b^{T}}}^{N} t_{i} \mathbf{x}_{i}^{T}$$



Now we have:  $\mathcal{X} = \mathbb{R}, \ \mathcal{Y} = \mathbb{R}, \ \phi_j(x) = x^j$ Given: data points  $(x_1, t_1), (x_2, t_2), \dots, (x_N, t_N)$ 















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Thus, we have: 
$$\sum_{i=1}^{N} \phi(x_i)\phi(x_i)^T = \Phi^T \Phi$$
where 
$$\Phi = \begin{pmatrix} \phi_0(x_1) & \phi_1(x_1) & \dots & \phi_{M-1}(x_1) \\ \phi_0(x_2) & \phi_1(x_2) & \dots & \phi_{M-1}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_N) & \phi_1(x_N) & \dots & \phi_{M-1}(x_N) \end{pmatrix}$$

$$\nabla E(\mathbf{w}) = \mathbf{w}^T \Phi^T \Phi - \mathbf{t}^T \Phi \implies \Phi^T \Phi \mathbf{w} = \Phi^T \mathbf{t}$$
"Normal Equation"
It follows:
$$\mathbf{w} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{t} \qquad \text{``Pseudoinverse''} \Phi^+$$



## **Computing the Pseudoinverse**

Mathematically, a pseudoinverse  $\Phi^+$  exists for every matrix  $\Phi$ .

However: If  $\Phi$  is (close to) singular the direct solution of  $\Phi$  is numerically unstable.

Therefore: Singular Value Decomposition (SVD) is used:  $\Phi = UDV^T$  where

- matrices U and V are orthogonal matrices
- D is a diagonal matrix

Then:  $\Phi^+ = VD^+U^T$  where  $D^+$  contains the

reciprocal of all non-zero elements of D



#### A Simple Example



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#### Varying the Sample Size



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#### **The Resulting Model Parameters**





#### **Other Basis Functions**

Other basis functions are possible:

Gaussian basis function:

$$\phi_j(x) := \exp\left(-\frac{(x-\mu_j)^2}{2s^2}\right)$$
 where  $\begin{array}{c} \mu_j \triangleq \text{mean val} \\ s \triangleq \text{scale} \end{array}$ 

Sigmoidal basis function:

$$\phi_j(x) := \sigma\left(\frac{x-\mu_j}{s}\right)$$
 where  $\sigma(a) = \frac{1}{1+\exp(-a)}$ 

In both cases a set of mean values is required. These define the locations of the basis functions.



#### **Gaussian Basis Functions**





#### **Sigmoidal Basis Functions**





#### **Observations**

- The higher the model complexity grows, the better is the fit to the data
- If the model complexity is too high, all data points are explained well, but the resulting model oscillates very much. It can not generalize well. This is called *overfitting*.
- By increasing the size of the data set (number of samples), we obtain a better fit of the model
- More complex models have larger parameters
   Problem: How can we find a good model complexity for a given data set with a fixed size?



#### Regularization

We observed that complex models yield large parameters, leading to oscillation. Idea:

Minimize the error function and the magnitude of the parameters simultaneously

We do this by adding a regularization term :

$$\tilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} \left( \mathbf{w}^{T} \boldsymbol{\phi}(x) - t_{i} \right)^{2} + \frac{\lambda}{2} \|\mathbf{w}\|^{2}$$

where  $\lambda$  rules the influence of the regularization.





#### Regularization

As above, we set the derivative to zero:

$$\nabla \tilde{E}(\mathbf{w}) = \sum_{i=1}^{N} \left( \mathbf{w}^{T} \boldsymbol{\phi}(x) - t_{i} \right) \boldsymbol{\phi}(x)^{T} + \lambda \mathbf{w}^{T} \doteq \mathbf{0}^{T}$$

$$\mathbf{w}^T \Phi^T \Phi + \lambda \mathbf{w}^T = \mathbf{t}^T \Phi \quad \Rightarrow \quad (\lambda I + \Phi^T \Phi) \mathbf{w} = \Phi^T \mathbf{t}$$

$$\mathbf{w} = (\lambda I + \Phi^T \Phi)^{-1} \Phi^T \mathbf{t}$$

With regularization, we can find a complex model for a small data set. However, the problem now is to find an appropriate regularization coefficient  $\lambda$ .



#### **Regularized Results**





#### The Problem from a Different View

Assume that *y* is affected by Gaussian noise :  $t = y(x, \mathbf{w}) + \epsilon$  where  $\epsilon \rightsquigarrow \mathcal{N}(.; 0, \sigma^2)$ 

Thus, we have  $p(t \mid x, \mathbf{w}, \sigma) = \mathcal{N}(t; y(x, \mathbf{w}), \sigma^2)$ 







**Aim:** we want to find the w that maximizes *p*.

 $p(t \mid x, \mathbf{w}, \sigma)$  is the *likelihood* of the measured data given a model. Intuitively:

Find parameters w that maximize the probability of measuring the already measured data t.

## "Maximum Likelihood Estimation"

We can think of this as fitting a model w to the data *t*. Note:  $\sigma$  is also part of the model and can be estimated. For now, we assume  $\sigma$  is known.



Given data points:  $(x_1, t_1), (x_2, t_2), \dots, (x_N, t_N)$ Assumption: points are drawn independently from *p*:

$$egin{aligned} p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \sigma) &= & \prod_{i=1}^N p(t_i \mid \mathbf{x}, \mathbf{w}, \sigma) \ &= & \prod_{i=1}^N \mathcal{N}(t_i; \mathbf{w}^T oldsymbol{\phi}(x_i), \sigma^2) \end{aligned}$$

where:  

$$\mathbf{x} = (x_1, x_2, \dots, x_N)$$
  
 $\mathbf{t} = (t_1, t_2, \dots, t_N)$ 

Instead of maximizing *p* we can also maximize its **logarithm** (monotonicity of the logarithm)



# The parameters that maximize the likelihood are equal to the minimum of the sum of squared errors





 $\mathbf{w}_{ML} := \arg \max_{\mathbf{w}} \ln p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \sigma) = \arg \min_{\mathbf{w}} E(\mathbf{w}) = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{t}$ The ML solution is obtained using the Pseudoinverse





#### **Maximum A-Posteriori Estimation**

So far, we searched for parameters w, that maximize the data likelihood. Now, we assume a Gaussian prior:

$$p(\mathbf{w} \mid \sigma_2) = \mathcal{N}(\mathbf{w}; \mathbf{0}, \sigma_2 I)$$

Using this, we can compute the *posterior* (Bayes):



### "Maximum A-Posteriori Estimation (MAP)"





#### **Maximum A-Posteriori Estimation**

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$$p(\mathbf{w} \mid \sigma_2) = \mathcal{N}(\mathbf{w}; \mathbf{0}, \sigma_2 I)$$

Using this, we can compute the *posterior* (Bayes):

$$p(\mathbf{w} \mid x, \mathbf{t}, \sigma_1, \sigma_2) \propto p(t \mid x, \mathbf{w}, \sigma_1) p(\mathbf{w} \mid \sigma_2)$$
  
ictly: 
$$p(t \mid x, \mathbf{w}, \sigma_1) p(\mathbf{w} \mid \sigma_2)$$

$$p(\mathbf{w} \mid x, \mathbf{t}, \sigma_1, \sigma_2) = \frac{1}{\int p(t \mid x, \mathbf{w}, \sigma_1) p(\mathbf{w} \mid \sigma_2) d\mathbf{w}}$$

but the denominator is independent of  $\mathbf{w}$  and we want to maximize p.

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#### **Maximum A-Posteriori Estimation**

$$\ln p(\mathbf{w} \mid x, \mathbf{t}, \sigma_1, \sigma_2) \propto \ln p(t \mid x, \mathbf{w}, \sigma_1) + \ln p(\mathbf{w} \mid \sigma_2)$$

$$(\cos t) - \frac{1}{\sigma_1^2} \sum_{i=1}^{N} (\mathbf{w}^T \boldsymbol{\phi}(x) - t_i)^2 \qquad (\cos t) - \frac{1}{2\sigma_2^2} \mathbf{w}^T \mathbf{w}$$

$$\propto -\frac{1}{\sigma_1^2} \left( \sum_{i=1}^N (\mathbf{w}^T \boldsymbol{\phi}(x) - t_i)^2 + \frac{\sigma_1^2}{\sigma_2^2} \mathbf{w}^T \mathbf{w} \right)$$

This is equal to the regularized error minimization. The MAP Estimate corresponds to a regularized error minimization where  $\lambda = (\sigma_1 / \sigma_2)^2$ 



### Summary

- Regression is a method to find a mathematical model (function) for a given data set
- Regression can be done by minimizing the sum of squared (SSE) errors, i.e. the distances to the data
- Maximum-likelihood estimation uses a probabilis-tic representation to fit a model into noisy data
- Maximum-likelihood under Gaussian noise is equivalent to SSE regression.
- Maximum-a-posteriori (MAP) estimation assumes a (Gaussian) prior on the model parameters
- MAP is solved by regularized regression





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## **Bayesian Linear Regression**

### **Bayesian Linear Regression**

- Using MAP, we can find optimal model parameters, but for practical applications two questions arise:
- What happens in the case of sequential data, i.e. the data points are observed subsequently?
- Can we model the probability of measuring a new data point, given all old data points? This is called the predictive distribution:





### When Bayes Meets Gauß

If we are given this:

$$\begin{array}{ll} \mathbf{p}(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}_1) & & \\ \mathbf{I}. \quad p(\mathbf{y} \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\mathbf{x} + \mathbf{b}, \boldsymbol{\Sigma}_2) & & \\ \end{array} \begin{array}{ll} \text{linear} \\ \text{dependency} \\ \text{on } \mathbf{x} \end{array} \end{array}$$

Then it follows (properties of Gaussians):

III. 
$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid A\mu + \mathbf{b}, \Sigma_2 + A\Sigma_1 A^T)$$
  
IV.  $p(\mathbf{x} \mid \mathbf{y}) = \mathcal{N}(\mathbf{x} \mid \Sigma(A^T \Sigma_2^{-1} (\mathbf{y} - \mathbf{b}) + \Sigma_1^{-1} \mu), \Sigma)$ 

where

$$\Sigma = (\Sigma_1^{-1} + A^T \Sigma_2^{-1} A)^{-1}$$

#### "Linear Gaussian Model"



#### **Sequential Data**

- **Given**: Prior mean  $\mathbf{m}_0$  and covariance  $S_0$ , noise covariance  $\sigma$   $p_0(\mathbf{w} \mid S_0) = \mathcal{N}(\mathbf{w}; \mathbf{m}_0, S_0)$
- **1.** Set i = 0
- 2. Observe data point  $(x_i, t_i)$
- 3. Formulate the likelihood  $p(t_i | x_i, \mathbf{w})$  as a function of **w** (= Gaussian with mean  $\phi(x_i)^T \mathbf{w}$  and covariance  $\sigma$ )
- 4. Multiply the likelihood with the prior  $p_i(\mathbf{w} \mid S_i)$  and normalize (= Gaussian with  $\mathbf{m}_{i+1}$  and  $S_{i+1}$ )
- 5. This results in a new prior  $p_{i+1}(\mathbf{w} \mid S_{i+1})$
- 6. Go back to 1. if there are still data points available



#### **Comparison: the Standard Bayes Filter**

$$Bel(x_t) = p(x_t \mid u_1, z_1, \dots, u_t, z_t)$$

(Bayes) = 
$$\eta p(z_t \mid x_t, u_1, z_1, \dots, u_t) p(x_t \mid u_1, z_1, \dots, u_t)$$

$$\begin{array}{ll} \text{(Markov)} &= \eta \; p(z_t \mid x_t) p(x_t \mid u_1, z_1, \dots, u_t) \\ \text{(Tot. prob.)} &= & \eta \; p(z_t \mid x_t) \int p(x_t \mid u_1, z_1, \dots, u_t, x_{t-1}) \\ & & p(x_{t-1} \mid u_1, z_1, \dots, u_t) dx_{t-1} \\ \text{(Markov)} &= \eta \; p(z_t \mid x_t) \int p(x_t \mid u_t, x_{t-1}) p(x_{t-1} \mid u_1, z_1, \dots, u_t) dx_{t-1} \\ \text{(Markov)} &= \eta \; p(z_t \mid x_t) \int p(x_t \mid u_t, x_{t-1}) p(x_{t-1} \mid u_1, z_1, \dots, z_{t-1}) dx_{t-1} \\ &= \eta \; p(z_t \mid x_t) \int p(x_t \mid u_t, x_{t-1}) \text{Bel}(x_{t-1}) dx_{t-1} \end{array}$$



#### **Comparison: the Standard Bayes Filter**

$$Bel(x_t) = p(x_t \mid u_1, z_1, \dots, u_t, z_t)$$

(Bayes) =  $\eta p(z_t \mid x_t, u_1, z_1, \dots, u_t) p(x_t \mid u_1, z_1, \dots, u_t)$ 

(Markov) =  $\eta \ p(z_t \mid x_t) p(x_t \mid u_1, z_1, \dots, u_t)$ 

#### **Note: Different Notation!**



### A Simple Example

- Our aim is to **fit a straight line** into a set of data points. Assume we have:
- Basis functions are equal to identity  $\phi(\mathbf{x}) = \mathbf{x}$
- Prior mean is zero, prior covariance  $\sigma_2^2 = 0.5$ , noise variance is  $\sigma_1^2 = 0.2^2$
- Ground truth is  $f(x, \mathbf{a}) = a_0 + a_1 x$  where  $a_1 = 0.5$ Data points are sampled from ground truth  $a_0 = -0.3$

Thus:

We want to recover  $a_0$  and  $a_1$  from the sequentially incoming data points  $(x_1, t_1), (x_2, t_2), \ldots$ 



#### No data points observed



From: C.M. Bishop





#### From: C.M. Bishop





#### Two data points observed



#### From: C.M. Bishop



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#### 20 data points observed



#### From: C.M. Bishop





#### **The Predictive Distribution**

We obtain the predictive distribution by integrating over all possible model parameters:

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$$p(t \mid x, \mathbf{t}, \mathbf{x}) = \int \underbrace{p(t \mid x, \mathbf{w}) p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}) d\mathbf{w}}_{\text{New data likelihood}} \qquad \text{Old data posterior}_{\text{Old data posterior}}$$
  
As before the posterior is prop. to the likelihood times the prior. But now, we don't maximize. The posterior can be computed analytically, as the prior is Gaussian.

$$p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}) = \mathcal{N}(\mathbf{w} \mid \mathbf{m}_N, S_N) \text{ where } \underbrace{S_N^{-1} = S_0^{-1} + \sigma^{-2} \Phi^T \Phi}_{\mathbf{W}_N = S_N(S_0^{-1} \mathbf{m}_0^{-1} + \sigma^{-2} \Phi^T \mathbf{t})}_{\mathbf{W}_N = S_N(S_0^{-1} \mathbf{m}_0^{-1} + \sigma^{-2} \Phi^T \mathbf{t})}$$

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#### **The Predictive Distribution**

Using formula III. from above (linear Gaussian),

$$p(t \mid x, \mathbf{t}, \mathbf{x}) = \int p(t \mid x, \mathbf{w}) p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}) d\mathbf{w}$$
$$= \int \mathcal{N}(t; \mathbf{w}^T \phi(x), \sigma) \mathcal{N}(\mathbf{w}; \mathbf{m}_N, S_N)$$

$$= \mathcal{N}(t; \mathbf{m}_N^T \phi(x), \sigma_N^2(x))$$

#### where

$$\sigma_N^2(x) = \sigma^2 + \phi(x)^T S_N \phi(x)$$



#### The Predictive Distribution (2)

 Example: Sinusoidal data, 9 Gaussian basis functions, 1 data point





#### **Predictive Distribution (3)**

 Example: Sinusoidal data, 9 Gaussian basis functions, 2 data points





### **Predictive Distribution (4)**

 Example: Sinusoidal data, 9 Gaussian basis functions, 4 data points





### **Predictive Distribution (5)**

 Example: Sinusoidal data, 9 Gaussian basis functions, 25 data points





### Summary

- Regression can be expressed as a least-squares problem
- To avoid overfitting, we need to introduce a **regularisation term** with an additional parameter  $\lambda$
- Regression without regularisation is equivalent to Maximum Likelihood Estimation
- Regression with regularisation is Maximum A-Posteriori
- Bayesian Linear Regression operates on sequential data and provides the predictive distribution
- When using Gaussian priors (and Gaussian noise), all computations can be done analytically

