

Fitting functions

Course of Machine Learning
Master Degree in Computer Science
University of Rome “Tor Vergata”

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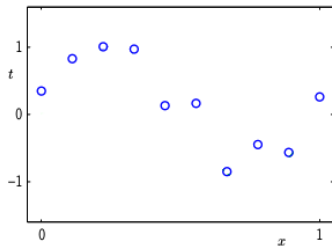
Example: fitting of polynomials

Problem

- ▶ A set of n observations of two variables $x, t \in \mathbb{R}$:
 $(x_1, t_1), \dots, (x_n, t_n)$ is available. We wish to exploit these observations to predict, for any value \tilde{x} of x , the corresponding unknown value of the target variable t
- ▶ The training set is a pair of vectors $\mathbf{x} = (x_1, \dots, x_n)^T$ and $\mathbf{t} = (t_1, \dots, t_n)^T$, related through an unknown rule (function)

Example: fitting of polynomials

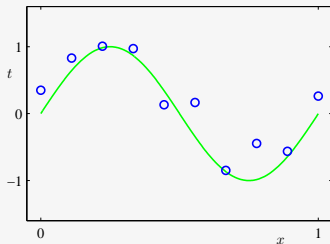
Example of a training set.



Example: fitting of polynomials

Training set

In this case, we assume that the (unknown) relation between x and t in the training set is provided by the function $t = \sin(2\pi x)$, with an additional gaussian noise with mean 0 and given variance σ^2 . Hence, $t_i = \sin(2\pi x_i) + \varepsilon_i$, with $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$.



Example: fitting of polynomials

Purpose

Guessing, or approximating as well as possible, the deterministic relation $t = \sin(2\pi x)$, on the basis of the analysis of data in the training set.

Example: fitting of polynomials

Approach

Let us approximate the unknown function through a suitable polynomial of given degree $M > 0$

$$y(x, \mathbf{w}) = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M = \sum_{j=0}^M w_jx^j$$

whose coefficients $\mathbf{w} = (w_0, w_1, \dots, w_M)^T$ are to be computed.

Linear models

$y(x, \mathbf{w})$ is a nonlinear function of x , but is a linear function (model) of \mathbf{w} .

Example: fitting of polynomials

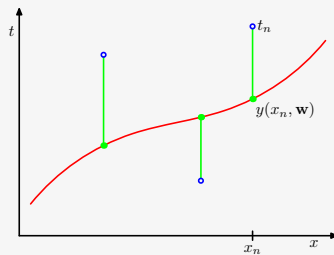
Parameter estimation

The values assigned to coefficients should minimize some **error function** (a.k.a. **cost function**), when applied to data in the training set (then, to x , t and w).

Example: fitting of polynomials

Least squares

A most widely adopted error function is **least squares**, i.e. the sum, for all items in the training set, of the (squared) difference between the value returned by the model and the target value.



$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^n (y(x_i, \mathbf{w}) - t_i)^2 = \frac{1}{2} \sum_{i=1}^n \left(w_0 + w_1 x_i + w_2 x_i^2 + \dots + w_M x_i^M \right)^2$$

Example: fitting of polynomials

Error minimization

- ▶ To minimize $E(\mathbf{w})$, set its derivative w.r.t. \mathbf{w} to $\mathbf{0}$
- ▶ $E(\mathbf{w})$ quadratic implies that its derivative is linear, hence that it is zero in one point w^*
- ▶ The resulting function is $y(x, \mathbf{w}^*)$

Example: fitting of polynomials

Derivative with respect to \mathbf{w}

The derivative w.r.t. \mathbf{w} is indeed a collection of derivatives. A linear system is then obtained:

$$\frac{\partial E(\mathbf{w})}{\partial w_0} = \sum_{i=1}^n (y(x_i, \mathbf{w}) - t_i) = 0$$

$$\frac{\partial E(\mathbf{w})}{\partial w_1} = \sum_{i=1}^n x_i (y(x_i, \mathbf{w}) - t_i) = 0$$

...

$$\frac{\partial E(\mathbf{w})}{\partial w_M} = \sum_{i=1}^n x_i^M (y(x_i, \mathbf{w}) - t_i) = 0$$

Example: fitting of polynomials

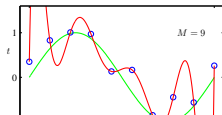
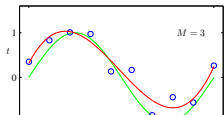
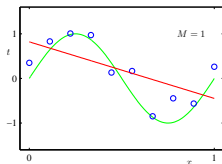
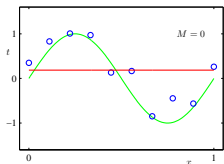
Derivative with respect to \mathbf{w}

Each of the $M + 1$ equations is linear w.r.t. each coefficient in \mathbf{w} . A linear system results, with $M + 1$ equations and $M + 1$ unknowns, which, in general and with the exceptions of degenerate cases, has precisely one solution.

Example: fitting of polynomials

Polynomial degree

- ▶ Example of **model selection**: assigning a value to M determines the model to be used, the choice of M implies the number of coefficients to be estimated
- ▶ increasing M allows to better approximate the training set items, decreasing the error
- ▶ if $M + 1 = n$ the model allows to obtain a null error (**overfitting**)



Example: fitting of polynomials

Overfitting

- ▶ The function $y(x, \mathbf{w})$ is derived from items in the training set, but should provide good predictions for other items.
- ▶ It should provide a suitable generalization to all items in the whole domain.
- ▶ If $y(x, \mathbf{w})$ is derived as a too much accurate depiction of the training set, it results into an unsuitable generalization to items not in the training set

Example: fitting of polynomials

Evaluation of the generalization

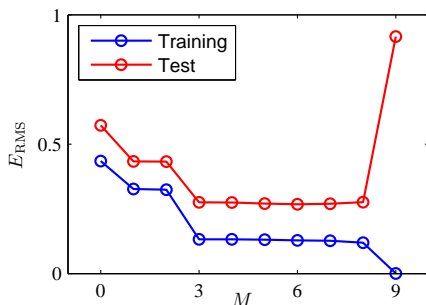
- ▶ Test set \mathbf{X}_{test} of 100 new items, generated by uniformly sampling x in $[0, 1,]$ and ε from $\mathcal{N}(0, \sigma^2)$, and computing $t = \sin 2\pi x + \varepsilon$
- ▶ For each M :
 - ▶ derives \mathbf{w}^* from the training set \mathbf{X}_{train}
 - ▶ compute the error $E(\mathbf{w}^*, \mathbf{X}_{test})$ on the test set, or the square root of its mean

$$E_{RMS}(\mathbf{w}^*, \mathbf{X}_{test}) = \sqrt{\frac{E(\mathbf{w}^*, \mathbf{X}_{test})}{|\mathbf{X}_{test}|}} = \sqrt{\frac{1}{2|\mathbf{X}_{test}|} \sum_{x \in \mathbf{X}_{test}} (y(x, \mathbf{w}) - t)^2}$$

- ▶ a lower value of $E_{RMS}(\mathbf{w}^*, \mathbf{X}_{test})$ denotes a good generalization

Example: fitting of polynomials

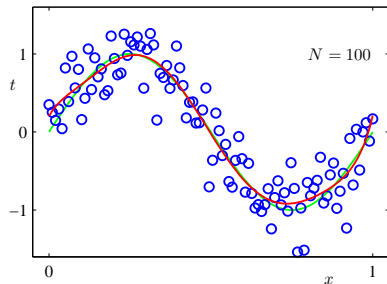
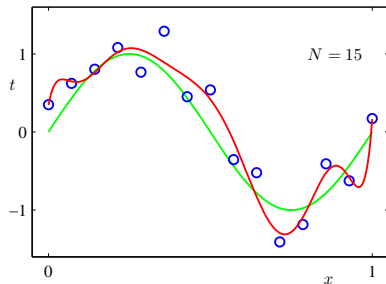
Plot of E_{RMS} w.r.t. M , on the training set and on the test set.



- ▶ As M increases, the error on the training set tends to 0.
- ▶ On the test set, the error initially decreases, since the higher complexity of the model allows to better represent the characteristics of the data set. Next, the error increases, since the model becomes too dependent from the training set: the noise component in t is too represented.

Example: fitting of polynomials

For a given model complexity (such as the degree in our example), overfitting decreases as the dimension of the dataset increases.



The larger the dataset, the higher the acceptable complexity of the model.

Example: fitting of polynomials

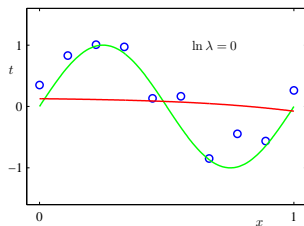
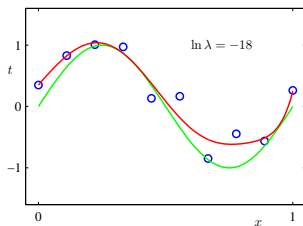
Use of **regularization** to limit complexity and overfitting.

- ▶ inclusion of a penalty term in the error function
- ▶ purpose: limiting the possible values of coefficients
- ▶ usually: limiting the modulus of the coefficient values

$$\begin{aligned}\tilde{E}(\mathbf{w}) &= \frac{1}{2} \sum_{i=1}^n (y(x_i, \mathbf{w}) - t_i)^2 + \frac{\lambda}{2} \sum_{k=0}^M w_k^2 \\ &= \frac{1}{2} \sum_{i=1}^n (y(x_i, \mathbf{w}) - t_i)^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2\end{aligned}$$

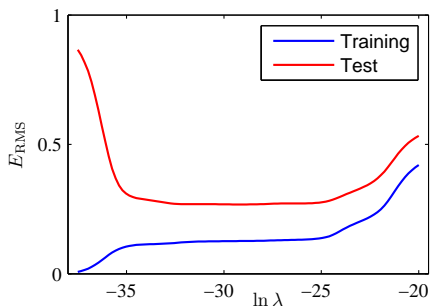
Example: fitting of polynomials

Dependence from the value of the hyperparameter λ .



Example: fitting of polynomials

Plot of the error w.r.t λ .



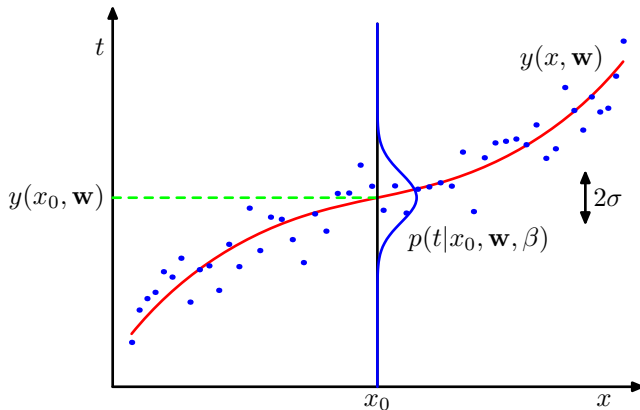
- ▶ Small λ : overfitting. Small error on the training set, large error on the test set.
- ▶ Large λ : the effect of data values decreases. Large error on both test and training sets.
- ▶ Intermediate λ . Intermediate error on training set, small error on test set.

Fitting of polynomial in terms of probability

Assume that, given an item \mathbf{x} , the corresponding unknown target t is normally distributed around the value returned by the model $\mathbf{w}^T \bar{\mathbf{x}}$, with a given variance $\sigma^2 = \beta^{-1}$:

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

Fitting of polynomial in terms of probability



Fitting of polynomial in terms of probability

An estimate of both β_{ML} and the coefficients \mathbf{w}_{ML} can be performed on the basis of the likelihood w.r.t. the assumed normal distribution:

$$L(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{i=1}^n \mathcal{N}(t_i|y(\mathbf{x}_i, \mathbf{w}), \beta^{-1})$$

Parameters \mathbf{w} and β can be estimated as the values which maximize the data likelihood, or its logarithm

$$l(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \sum_{i=1}^n \log \mathcal{N}(t_i|y(\mathbf{x}_i, \mathbf{w}), \beta^{-1})$$

which results into

$$\begin{aligned} l(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) &= \sum_{i=1}^n \log \left(\frac{\sqrt{\beta}}{\sqrt{2\pi}} e^{-\frac{\beta}{2}(t_i - y(\mathbf{x}_i, \mathbf{w}))^2} \right) \\ &= - \sum_{i=1}^n \frac{\beta}{2} (t_i - y(\mathbf{x}_i, \mathbf{w}))^2 + \frac{n}{2} \log \beta - \frac{n}{2} \log(2\pi) \\ &= - \frac{\beta}{2} \sum_{i=1}^n (t_i - y(\mathbf{x}_i, \mathbf{w}))^2 + \frac{n}{2} \log \beta + \text{cost} \end{aligned}$$

Fitting of polynomial in terms of probability

The maximization w.r.t. \mathbf{w} is performed by determining a maximum w.r.t. \mathbf{w} of the function

$$-\frac{1}{2} \sum_{i=1}^n (t_i - y(\mathbf{x}_i, \mathbf{w}))^2$$

this is equivalent to minimizing the least squares sum.

The maximization w.r.t. the **precision** β is done by setting to 0 the corresponding derivative

$$\frac{\partial l(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta)}{\partial \beta} = -\frac{1}{2} \sum_{i=1}^n (t_i - y(\mathbf{x}_i, \mathbf{w}))^2 + \frac{n}{2\beta}$$

which results into

$$\beta_{ML}^{-1} = \frac{1}{n} \sum_{i=1}^n (t_i - y(\mathbf{x}_i, \mathbf{w}))^2$$

Fitting of polynomial in terms of probability

As a side result, the parameter estimate provides a **predictive distribution** of t given \mathbf{x} , that is the (gaussian) distribution of the target value for a given item \mathbf{x} .

$$p(t|\mathbf{x}; \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}) = \sqrt{\frac{\beta_{ML}}{2\pi}} e^{-\frac{\beta_{ML}}{2}(t-y(\mathbf{x}, \mathbf{w}_{ML}))^2}$$

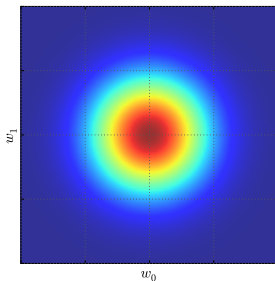
Fitting of polynomial in terms of probability

- ▶ In the maximum likelihood framework parameters are considered as (unknown) values to determine with the best possible precision (frequentist approach).
- ▶ An alternative framework (bayesian) looks at parameters as random variables, whose probability distribution has to be derived.

Fitting of polynomial in terms of probability

Prior distribution of parameters: gaussian with mean $\mathbf{0}$ and diagonal covariance matrix with variance equal to the inverse of **hyperparameter** α

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



Fitting of polynomial in terms of probability

From Bayes rule, the distribution of \mathbf{w} , given the observed training set (\mathbf{X}, \mathbf{t}) , is proportional to the product of the prior distribution and the likelihood of the training set

$$\begin{aligned} p(\mathbf{w}|\mathbf{X}, \mathbf{t}; \alpha, \beta) &= \propto p(\mathbf{t}|\mathbf{X}, \mathbf{w}; \beta) p(\mathbf{w}|\alpha) \\ &= \prod_{i=1}^n \left(\frac{\sqrt{\beta}}{\sqrt{2\pi}} e^{-\frac{\beta}{2}(t_i - y(\mathbf{x}_i, \mathbf{w}))^2} \right) \left(\frac{\alpha}{2\pi} \right)^{\frac{M+1}{2}} e^{-\frac{\alpha}{2} \mathbf{w}^T \mathbf{w}} \end{aligned}$$

Computing the maximum of the posterior distribution (MAP): equivalent to the maximization of the corresponding logarithm

$$-\frac{\beta}{2} \sum_{i=1}^n (t_i - y(\mathbf{x}_i, \mathbf{w}))^2 + \frac{n}{2} \log \beta - \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \frac{M+1}{2} \log \frac{\alpha}{2\pi} + \text{const}$$

The value \mathbf{w}_{MAP} which maximize the probability (mode of the distribution) also minimizes

$$\frac{\beta}{2} \sum_{i=1}^n (t_i - y(\mathbf{x}_i, \mathbf{w}))^2 + \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} = \beta \left(\frac{1}{2} \sum_{i=1}^n (t_i - y(\mathbf{x}_i, \mathbf{w}))^2 + \frac{\alpha}{2\beta} \|\mathbf{w}\|^2 \right)$$

The ratio $\frac{\alpha}{\beta}$ corresponds to a regularization hyperparameter.

Fitting of polynomial in terms of probability

The same considerations of ML apply here for what concerns deriving the **predictive distribution** of t given \mathbf{x} , which results now

$$p(t|\mathbf{x}; \mathbf{w}, \beta_{MAP}) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta_{MAP}^{-1}) = \sqrt{\frac{\beta_{MAP}}{2\pi}} e^{-\frac{\beta_{MAP}}{2}(t-y(\mathbf{x}, \mathbf{w}_{MAP}))^2}$$

where, as it is easy to see, $\beta_{MAP} = \beta_{ML}$

Bayesian fitting

A **pure bayesian** approach to this problem aims to derive the predictive distribution of t given \mathbf{x} from the training set (\mathbf{X}, \mathbf{t}) directly, without assuming any type of distribution and then performing some kind of evaluation of the corresponding parameters.

From the basic properties of probabilities,

$$\begin{aligned} p(t|\mathbf{x}; \mathbf{X}, \mathbf{t}) &= \int p(t, \mathbf{w}|\mathbf{x}; \mathbf{X}, \mathbf{t}) d\mathbf{w} \\ &= \int p(t|\mathbf{w}, \mathbf{x}; \mathbf{X}, \mathbf{t}) p(\mathbf{w}|\mathbf{x}; \mathbf{X}, \mathbf{t}) d\mathbf{w} \\ &= \int p(t|\mathbf{w}, \mathbf{x}) p(\mathbf{w}|\mathbf{X}, \mathbf{t}) d\mathbf{w} \end{aligned}$$

since \mathbf{w} is independent from \mathbf{x} , and, once \mathbf{w} is given, t is independent from \mathbf{X} and \mathbf{t} . That is, $\mathbf{x} \perp\!\!\!\perp \mathbf{w}$, $t \perp\!\!\!\perp \mathbf{X}|\mathbf{w}$, $t \perp\!\!\!\perp \mathbf{t}|\mathbf{w}$.

Bayesian fitting

We shall see later that, if we assume that:

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

$$p(\mathbf{w}; \alpha)$$

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

are all gaussians, then the evidence is gaussian too.

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

with mean and variance deriving from the training set as follows

$$m(\mathbf{x}) = \beta \mathbf{x}^T \mathbf{S} \sum_{i=1}^n \mathbf{x}_i \mathbf{t}_i$$

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

$$\mathbf{S} = \alpha \mathbf{I} + \beta \sum_{i=1}^n \mathbf{x} \mathbf{x}^T$$

Bayesian fitting

- ▶ The mean is clearly a function $m(x)$ of x .
- ▶ The variance is also dependent from x . The term β^{-1} is independent from x and represents the uncertainty in the knowledge of t .

