Sapienza University of Rome

Master in Artificial Intelligence and Robotics
Master in Engineering in Computer Science

Machine Learning

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8. Linear models for regression

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Overview

- Linear models for regression
- Maximum likelihood and Least squares
- Sequential learning
- Regularization

References

C. Bishop. Pattern Recognition and Machine Learning. Sect. 3.1

Linear Models for Regression

Learning a function $f : X \to Y$, with

- $X \subseteq \Re^d$
- $Y = \Re$

from data set $D = \{(\mathbf{x}_n, t_n)_{n=1}^N\}$

Linear Models for Regression

Define a model $y(\mathbf{x};\mathbf{w})$ with parameters $\mathbf{w}$ to approximate the target function f. → linear

Linear model for linear function

linear comb.

$$y(\mathbf{x};\mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d = \mathbf{w}^T\mathbf{x}$$

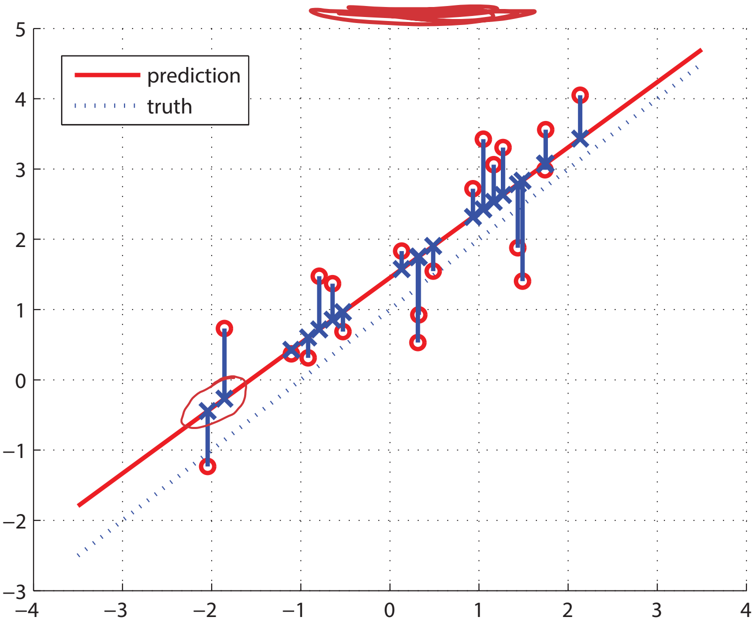
no ~ because it includes $w_0 \cdot 1$.

$$\text{with } \mathbf{x} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix} \text{ and } \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

Why 1? Exam at 20:4?

Example: 2D line fitting

$$y = w_0 + w_1 x_1$$



Linear Models for Regression

Linear Basis Function Models

Using nonlinear functions of input variables:

the same of classification: transform input data.

$$y(\mathbf{x};\mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}),$$

NO NEED TO BE INVERTIBLE

$$\text{with } \mathbf{w} = \begin{bmatrix} w_0 \\ \vdots \\ w_{M-1} \end{bmatrix} \quad \phi(\mathbf{x}) = \begin{bmatrix} \phi_0(\mathbf{x}) \\ \vdots \\ \phi_{M-1}(\mathbf{x}) \end{bmatrix}, \text{ and } \phi_0(\mathbf{x}) = 1.$$

Basis function

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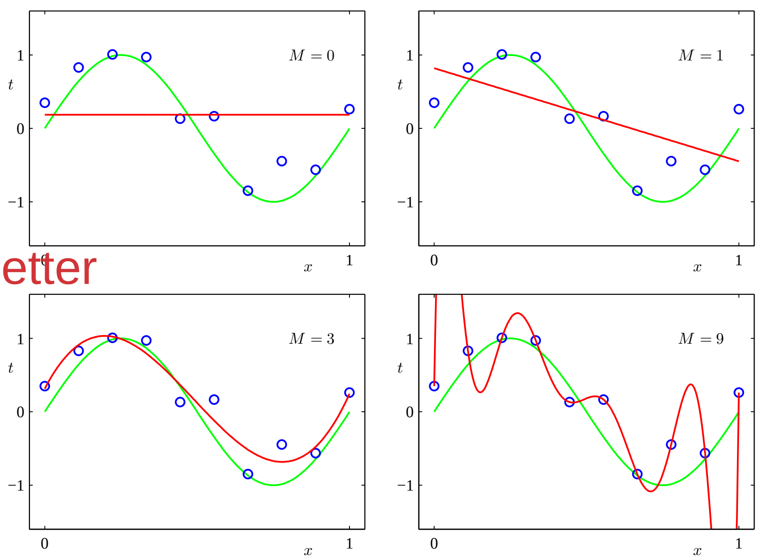
- Still linear in the parameters $\mathbf{w}$!

Example: Polynomial curve fitting

PROBLEM IS TO FIND W.

$$y = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

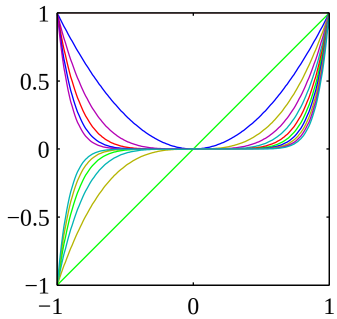
Right degree fit better



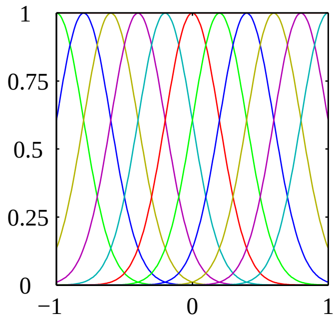
Too high degree for polynomial you will overfit, 0 training error, but very high test error.

Linear Regression Basis Functions

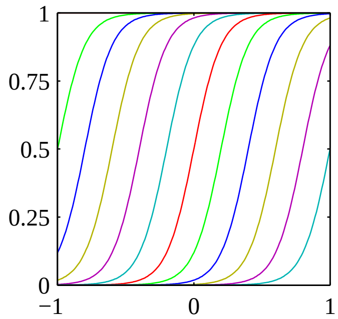
Examples of basis functions



Polynomial



Radial



Sigmoid / Tanh

Linear Regression - Algorithms

Maximum likelihood and least squares

Target value t is given by $y(\mathbf{x}; \mathbf{w})$ affected by additive noise ϵ

$$t = y(\mathbf{x}; \mathbf{w}) + \epsilon$$ noise (error)

Assume Gaussian noise $P(\epsilon|\beta) = \mathcal{N}(\epsilon|0, \beta^{-1})$, with precision (inverse variance) β.

centered at 0

We have:

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

Linear Regression - Algorithms

Assume observations independent and identically distributed (i.i.d.)

We seek the maximum of the likelihood function:

find w that max this P.

$$P(\{t_1, \ldots, t_N\}|\mathbf{x}_1, \ldots, \mathbf{x}_n, \boxed{\mathbf{w}}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|\mathbf{w}^T\phi(\mathbf{x}_n), \beta^{-1}).$$

or equivalently:

$$\ln P(\{t_1, \ldots, t_N\}|\mathbf{x}_1, \ldots, \mathbf{x}_N, \mathbf{w}, \beta) = \sum_{n=1}^{N} \ln \mathcal{N}(t_n|\mathbf{w}^T\phi(\mathbf{x}_n), \beta^{-1})$$

Squared err.

Maximizing the probability means minimizing error

$$= -\beta \underbrace{\frac{1}{2}\sum_{n=1}^{N}[t_n - \mathbf{w}^T\phi(\mathbf{x}_n)]^2}_{E_D(\mathbf{w})} - \frac{N}{2}\ln(2\pi\beta^{-1}).$$

Linear Regression - Algorithms

Maximum likelihood (zero-mean Gaussian noise assumption)

$$\mathrm{argmax}\, P(\{t_1, \ldots, t_N\}|\mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{w}, \beta)$$

corresponds to least square error minimization

$$\mathrm{argmin}\, E_D(\mathbf{w}) = \mathrm{argmin}\, \frac{1}{2}\sum_{n=1}^{N}[t_n - \mathbf{w}^T\phi(\mathbf{x}_n)]^2$$

Linear Regression - Algorithms

Note:

$$E_D(\mathbf{w}) = \frac{1}{2}(\mathbf{t} - \mathbf{\Phi w})^T(\mathbf{t} - \mathbf{\Phi w}),$$

$$\text{with } \mathbf{t} = \begin{bmatrix} t_1 \\ \vdots \\ t_N \end{bmatrix} \text{ and } \mathbf{\Phi} = \begin{bmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{bmatrix}.$$

Optimality condition:

$$\nabla E_D = 0 \iff \mathbf{\Phi}^T\mathbf{\Phi w} = \mathbf{\Phi}^T\mathbf{t}.$$

Why gradient instead of the solution using phi matrix? If the input is too large this may be not practical

Hence:

$$\mathbf{w}_{ML} = \underbrace{(\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T}_{\mathbf{\Phi}^\dagger:\ \text{pseudo-inverse}}\ \mathbf{t}.$$

Linear Regression - Algorithms

Sequential Learning

Stochastic gradient descent algorithm:

$$\hat{\mathbf{w}} \leftarrow \hat{\mathbf{w}} - \eta \nabla E_n$$

η: learning rate parameter

Therefore:

$$\hat{\mathbf{w}} \leftarrow \hat{\mathbf{w}} + \eta\,[t_n - \hat{\mathbf{w}}^T\phi(\mathbf{x}_n)]\,\phi(\mathbf{x}_n)$$

Algorithm converges for suitable small values of η.

Linear Regression - Regularization

Regularization is a technique to control over-fitting.

$$\operatorname{argmin} \overbrace{E_D(\mathbf{w})}^{\text{error}} + \overbrace{\lambda E_W(\mathbf{w})}^{\text{artificial error}}$$

with $\lambda > 0$ being the regularization factor

A common choice:

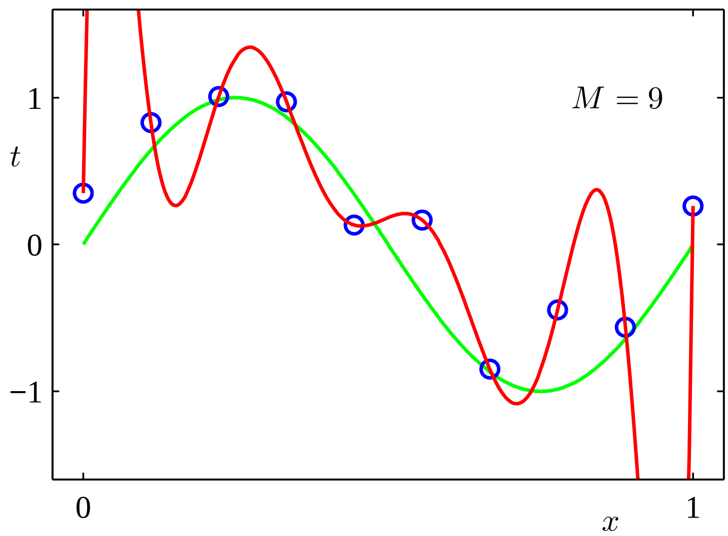
$$E_W(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w}.$$

Other choices:

$$E_W(\mathbf{w}) = \sum_{j=0}^{M-1} |w_j|^q.$$

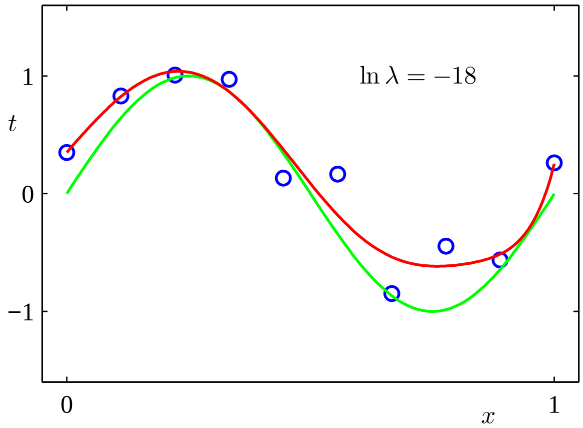
Linear Regression - Regularization

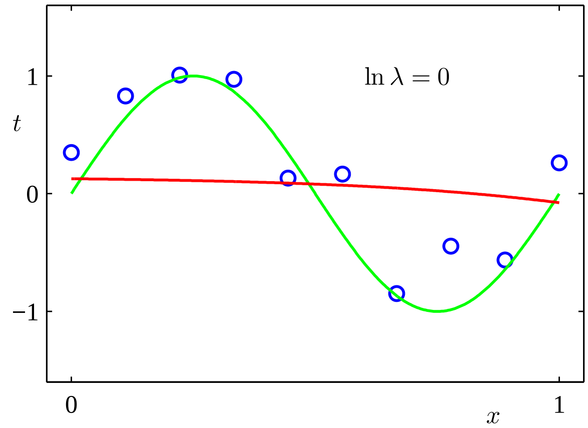
$$\operatorname{argmin} E_D(\mathbf{w})$$



Linear Regression - Regularization

$$\operatorname{argmin} \; E_D(\mathbf{w}) + \overbrace{\lambda \frac{1}{2}\mathbf{w}^T\mathbf{w}}^{\lambda E_W}$$





Linear Regression - Multiple outputs

$$\mathbf{y}(\mathbf{x}; \mathbf{W}) = \mathbf{W}^T \phi(\mathbf{x})$$

Target variable is given by:

$$\mathbf{T} = \mathbf{y}(\mathbf{x}; \mathbf{W}) + \epsilon$$

with $P(\boldsymbol{\epsilon}|\beta) = \mathcal{N}(\boldsymbol{\epsilon}|0, \beta^{-1}\mathbf{I})$.

Similarly with before we obtain:

$$\mathbf{W}_{ML} = (\Phi^T\Phi)^{-1}\Phi^T\mathbf{T}.$$