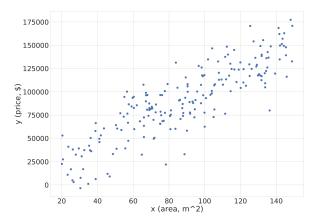
Section 1

Basic Linear Regression

Example: Housing price prediction

Given is a dataset $\mathcal{D}=\{(x_i,y_i)\}_{i=1}^N$, of house areas x_i and corresponding prices y_i .



How do we estimate a price of a new house with area x_{new} ?

Regression problem

Given

observations ¹

$$oldsymbol{X} = \{oldsymbol{x}_1, oldsymbol{x}_2, \dots, oldsymbol{x}_N\}$$
, $oldsymbol{x}_i \in \mathbb{R}^D$

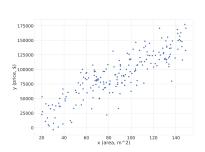
• targets

$$\mathbf{y} = \{y_1, y_2, \dots, y_N\}, \quad y_i \in \mathbb{R}$$

Find

• Mapping $f(\cdot)$ from inputs to targets

$$y_i \approx f(\boldsymbol{x}_i)$$



 $^{^1\}text{A}$ common way to represent the samples is as a data matrix $\pmb{X} \in \mathbb{R}^{N \times D}$, where each row represents one sample.

Linear model

Target y is generated by a deterministic function f of x plus noise

$$y_i = f(\mathbf{x}_i) + \epsilon_i, \qquad \epsilon_i \sim \mathcal{N}(0, \beta^{-1})$$
 (1)

Let's choose f(x) to be a linear function

$$f_{\mathbf{w}}(\mathbf{x}_i) = w_0 + w_1 x_{i1} + w_2 x_{i2} + \dots + w_D x_{iD}$$
 (2)

$$= w_0 + \boldsymbol{w}^T \boldsymbol{x}_i \tag{3}$$

From now we will always assume that the bias term is absorbed into the $oldsymbol{x}$ vector

Linear Regression 6

Absorbing the bias term

The linear function is given by

$$f_{\mathbf{w}}(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_D x_D \tag{4}$$

$$= w_0 + \boldsymbol{w}^T \boldsymbol{x} \tag{5}$$

Here w_0 is called bias or offset term. For simplicity, we can "absorb" it by prepending a 1 to the feature vector x and respectively adding w_0 to the weight vector w:

$$\tilde{\boldsymbol{x}} = (1, x_1, ..., x_D)^T$$
 $\tilde{\boldsymbol{w}} = (w_0, w_1, ..., w_D)^T$

The function $f_{\boldsymbol{w}}$ can compactly be written as $f_{\boldsymbol{w}}(\boldsymbol{x}) = \tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{x}}$.

To unclutter the notation, we will assume the bias term is always absorbed and write w and x instead of \tilde{w} and \tilde{x} .

Now, how do we choose the "best" w that fits our data?

Linear Regression 7 and A

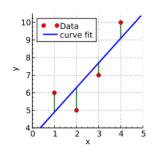
Error function

Error function gives a measure of "misfit" between our model (parametrized by w) and observed data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$.

Standard choice - least squares (LS) function

$$E_{LS}(\boldsymbol{w}) = \frac{1}{2} \sum_{i=1}^{N} (f_{\boldsymbol{w}}(\boldsymbol{x}_i) - y_i)^2$$
 (6)

$$= \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{x}_{i} - y_{i})^{2}$$
 (7)



Objective

Find the optimal weight vector w^\star that minimizes the error

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{x}} E_{\mathrm{LS}}(\boldsymbol{w}) \tag{8}$$

$$= \underset{\boldsymbol{w}}{\operatorname{arg\,min}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{x}_{i}^{T} \boldsymbol{w} - y_{i})^{2}$$
(9)

By stacking the observations $oldsymbol{x}_i$ as rows of the matrix $oldsymbol{X} \in \mathbb{R}^{N imes D}$

$$= \underset{\boldsymbol{w}}{\operatorname{arg\,min}} \frac{1}{2} (\boldsymbol{X} \boldsymbol{w} - \boldsymbol{y})^{T} (\boldsymbol{X} \boldsymbol{w} - \boldsymbol{y})$$
 (10)

Optimal solution

To find the minimum of the function $E(\boldsymbol{w})$, compute the gradient $\nabla_{\boldsymbol{w}} E(\boldsymbol{w})$:

$$\nabla_{\boldsymbol{w}} E_{\mathrm{LS}}(\boldsymbol{w}) = \nabla_{\boldsymbol{w}} \frac{1}{2} (\boldsymbol{X} \boldsymbol{w} - \boldsymbol{y})^{T} (\boldsymbol{X} \boldsymbol{w} - \boldsymbol{y})$$
(11)

$$= \nabla_{\boldsymbol{w}} \frac{1}{2} \left(\boldsymbol{w}^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{w} - 2 \boldsymbol{w}^T \boldsymbol{X}^T \boldsymbol{y} + \boldsymbol{y}^T \boldsymbol{y} \right)$$
(12)

$$= \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{w} - \boldsymbol{X}^T \boldsymbol{y} \tag{13}$$

Optimal solution

Now set the gradient to zero and solve for ${m w}$ to obtain the minimizer 2

$$\boldsymbol{X}^T \boldsymbol{X} \boldsymbol{w} - \boldsymbol{X}^T \boldsymbol{y} \stackrel{!}{=} 0 \tag{14}$$

This leads to the so-called normal equation of the least squares problem

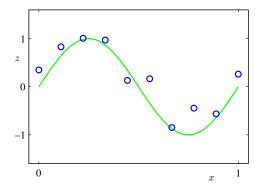
$$w^* = \underbrace{(X^\mathsf{T} X)^{-1} X^\mathsf{T}}_{=X^\dagger} y \tag{15}$$

 X^\dagger is called Moore-Penrose pseudo-inverse of X (because for an invertible square matrix, $X^\dagger = X^{-1}$).

²Because Hessian $\nabla_{\boldsymbol{w}}\nabla_{\boldsymbol{w}}E(\boldsymbol{w})$ is positive (semi)definite \rightarrow see *Optimization*

Nonlinear dependency in data

What if the dependency between y and x is not linear?



Data generating process:
$$y_i = \sin(2\pi x_i) + \epsilon, \qquad \epsilon \sim \mathcal{N}(0, \beta^{-1})$$

For this example assume that data dimensionality $D=1\,$

Polynomials

Solution: Polynomials are universal function approximators, so we can define \boldsymbol{f} as

$$f_{\mathbf{w}}(x) = w_0 + \sum_{j=1}^{M} w_j x^j$$
 (16)

Or more generally

$$= w_0 + \sum_{j=1}^{M} w_j \phi_j(x)$$
 (17)

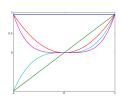
Define $\phi_0 = 1$

$$= \boldsymbol{w}^T \boldsymbol{\phi}(x) \tag{18}$$

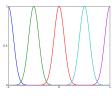
The function f is still linear in w (despite not being linear in x)!

Typical basis functions

$$\phi_j(x) = x^j$$



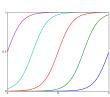
$$\phi_j(x) = e^{\frac{-(x-\mu_j)^2}{2s^2}}$$



Logistic Sigmoid

$$\phi_j(x) = \sigma(\frac{x - \mu_j}{s}),$$

where
$$\sigma(a) = \frac{1}{1+\mathrm{e}^{-a}}$$



Linear basis function model

Prediction for one sample

$$f_{\boldsymbol{w}}(\boldsymbol{x}) = w_0 + \sum_{j=1}^{M} w_j \phi_j(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})$$
(19)

Using the same least squares error function as before

$$E_{LS}(\boldsymbol{w}) = \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2}$$

$$= \frac{1}{2} (\boldsymbol{\Phi} \boldsymbol{w} - \boldsymbol{y})^{T} (\boldsymbol{\Phi} \boldsymbol{w} - \boldsymbol{y})$$
(20)

with

$$oldsymbol{\Phi} = \left(egin{array}{cccc} \phi_0(oldsymbol{x}_1) & \phi_1(oldsymbol{x}_1) & \dots & \phi_M(oldsymbol{x}_1) \ \phi_0(oldsymbol{x}_2) & \phi_1(oldsymbol{x}_2) & & dots \ dots & dots & \ddots & \ \phi_0(oldsymbol{x}_N) & \phi_1(oldsymbol{x}_N) & \dots & \phi_M(oldsymbol{x}_N) \end{array}
ight) \in \mathbb{R}^{N imes (M+1)}$$

being the design matrix of ϕ .

Optimal solution

Recall Equation 10 - we have the same expression except that data matrix $X \in \mathbb{R}^{N \times D}$ is replaced by design matrix $\Phi \in \mathbb{R}^{N \times (M+1)}$

$$E_{LS}(\boldsymbol{w}) = \frac{1}{2} (\boldsymbol{\Phi} \boldsymbol{w} - \boldsymbol{y})^T (\boldsymbol{\Phi} \boldsymbol{w} - \boldsymbol{y})$$
 (22)

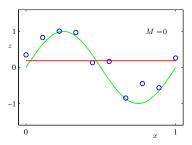
This means that the optimal weights $oldsymbol{w}^*$ can be obtained in a similar way

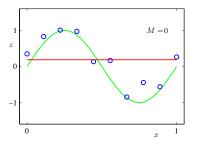
$$\boldsymbol{w}^* = (\boldsymbol{\Phi}^\mathsf{T} \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^\mathsf{T} \boldsymbol{y} \tag{23}$$

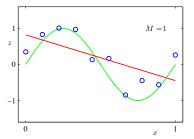
$$= \Phi^{\dagger} y \tag{24}$$

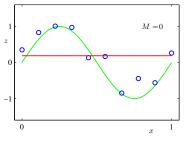
Compare this to Equation 15:

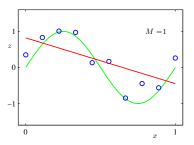
$$\boldsymbol{w}^* = (\boldsymbol{X}^\mathsf{T} \boldsymbol{X})^{-1} \boldsymbol{X}^\mathsf{T} \boldsymbol{y} \tag{25}$$

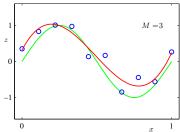


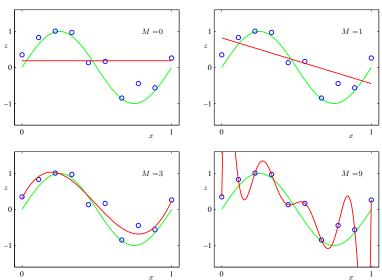


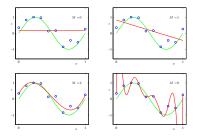


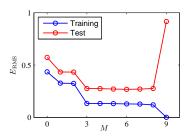




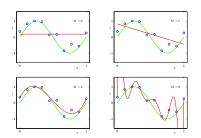








One valid solution is to choose ${\cal M}$ using the standard train-validation split approach.



	M = 0	M = 1	M = 6	M = 9
w_0^{\star}	0.19	0.82	0.31	0.35
w_1^{\star}		-1.27	7.99	232.37
w_2^{\star}			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^{\star}				-231639.30
w_5^{\star}				640042.26
w_6^{\star}				-1061800.52
w_7^*				1042400.18
w_8^{\star}				-557682.99
w_9^{\star}				125201.43

We also make another observation: overfitting occurs when the coefficients \boldsymbol{w} become large.

What if we penalize large weights?

Controlling overfitting with regularization

Least squares loss function with L2 regularization (also called ridge regression)

$$E_{\text{ridge}}(\boldsymbol{w}) = \frac{1}{2} \sum_{i=1}^{N} \left[\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i} \right]^{2} + \frac{\lambda}{2} \|\boldsymbol{w}\|_{2}^{2}$$
 (26)

Where,

- $\| oldsymbol{w} \|_2^2 \equiv oldsymbol{w}^T oldsymbol{w} = w_0^2 + w_1^2 + w_2^2 + \dots + w_M^2$ L2 norm
- ullet $\lambda-$ regularization strength

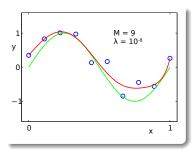
Controlling overfitting with regularization

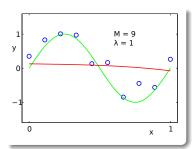
Least squares loss function with L2 regularization (also called ridge regression)

$$E_{\text{ridge}}(\boldsymbol{w}) = \frac{1}{2} \sum_{i=1}^{N} \left[\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i} \right]^{2} + \frac{\lambda}{2} \|\boldsymbol{w}\|_{2}^{2}$$
 (26)

Where,

- $\| \boldsymbol{w} \|_2^2 \equiv \boldsymbol{w}^T \boldsymbol{w} = w_0^2 + w_1^2 + w_2^2 + \dots + w_M^2$ L2 norm
- λ regularization strength





Larger regularization strength λ leads to smaller weights w

Section 2

Probabilistic Linear Regression

Probabilistic formulation

Remember from our problem definition at the start of the lecture,

$$y_i = f_{\boldsymbol{w}}(\boldsymbol{x}_i) + \underline{\epsilon_i}$$

Noise has zero-mean Gaussian distribution with a fixed precision $\beta = \frac{1}{\sigma^2}$

$$\epsilon_i \sim \mathcal{N}(0, \beta^{-1})$$

This implies that the distribution of the targets is

$$y_i \sim \mathcal{N}(f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta^{-1})$$

Remember: any function can be represented as $f_{m{w}}(m{x}_i) = m{w}^T \phi(m{x}_i)$

Maximum likelihood

Likelihood of a single sample

$$p(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta) = \mathcal{N}(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta^{-1})$$
(27)

Assume that the samples are drawn i.i.d.

 \implies likelihood of the entire dataset $\mathcal{D} = \{ oldsymbol{X}, oldsymbol{y} \}$ is

$$p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) = \prod_{i=1}^{N} p(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta)$$
 (28)

We can now use the same approach we used in previous lecture - maximize the likelihood w.r.t. ${\pmb w}$ and ${\pmb \beta}$

$$\boldsymbol{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}} = \underset{\boldsymbol{w}, \beta}{\operatorname{arg\,max}} p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)$$
 (29)

Maximum likelihood

Like in the coin flip example, we can make a few simplifications

$$\mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}} = \operatorname*{arg\,max}_{\mathbf{w},\beta} p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}, \beta)$$

$$\mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}} = \operatorname*{arg\,max}_{\mathbf{w},\beta} p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}, \beta)$$

$$(30)$$

$$= \operatorname*{arg\,max}_{\boldsymbol{w},\beta} \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \tag{31}$$

$$= \underset{\boldsymbol{w},\beta}{\operatorname{arg\,min}} - \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)$$
 (32)

Let's denote this quantity as maximum likelihood error function that we need to minimize

$$E_{\mathrm{ML}}(\boldsymbol{w}, \beta) = -\ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)$$
(33)

Linear Regression 33 and Analytic

Maximum likelihood

Simplify the error function

$$E_{\text{ML}}(\boldsymbol{w}, \beta) = -\ln \left[\prod_{i=1}^{N} \mathcal{N}(y_i \mid f_{\boldsymbol{w}}(\boldsymbol{x}_i), \beta^{-1}) \right]$$

$$= -\ln \left[\prod_{i=1}^{N} \sqrt{\frac{\beta}{2\pi}} \exp\left(-\frac{\beta}{2} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2\right) \right]$$

$$= -\sum_{i=1}^{N} \ln \left[\sqrt{\frac{\beta}{2\pi}} \exp\left(-\frac{\beta}{2} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2\right) \right]$$

$$= \frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 - \frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi$$
(37)

Optimizing log-likelihood w.r.t. $oldsymbol{w}$

$$\mathbf{w}_{\mathrm{ML}} = \operatorname*{arg\,min}_{\mathbf{w}} E_{\mathrm{ML}}(\mathbf{w}, \beta) \tag{38}$$

$$= \underset{\boldsymbol{w}}{\operatorname{arg min}} \left[\frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2} \underbrace{-\frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi}_{= \text{ const}} \right]$$
(39)

$$= \arg\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2}$$

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$$= \arg\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2}$$

$$= \arcsin\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2}$$

$$= -2 \operatorname{constant} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2}$$

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$$= \underset{\boldsymbol{w}}{\operatorname{arg\,min}} E_{\mathrm{LS}}(\boldsymbol{w}) \tag{41}$$

Optimizing log-likelihood w.r.t. $oldsymbol{w}$

$$\mathbf{w}_{\mathrm{ML}} = \operatorname*{arg\,min}_{\mathbf{w}} E_{\mathrm{ML}}(\mathbf{w}, \beta) \tag{38}$$

$$= \underset{\boldsymbol{w}}{\operatorname{arg min}} \left[\frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2} - \frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi \right]$$
(39)

$$= \underset{\boldsymbol{w}}{\operatorname{arg\,min}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2}$$

$$\underset{\text{least squares error fn!}}{}$$

$$(40)$$

$$= \underset{\boldsymbol{w}}{\arg\min} E_{\mathrm{LS}}(\boldsymbol{w}) \tag{41}$$

Maximizing the likelihood is equivalent to minimizing the least squares error function!

$$\boldsymbol{w}_{\mathrm{ML}} = (\boldsymbol{\Phi}^{\mathsf{T}} \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^{\mathsf{T}} \boldsymbol{y} = \boldsymbol{\Phi}^{\dagger} \boldsymbol{y} \tag{42}$$

Optimizing log-likelihood w.r.t. β

Plug in the estimate for ${m w}$ and minimize w.r.t. ${m eta}$

$$\beta_{\rm ML} = \underset{\beta}{\arg\min} E_{\rm ML}(\boldsymbol{w}_{\rm ML}, \beta) \tag{43}$$

$$= \underset{\beta}{\operatorname{arg\,min}} \left[\frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}_{\mathrm{ML}}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2} - \frac{N}{2} \ln \beta + \frac{N}{2} \ln 2\pi \right]$$
 (44)

Take derivative w.r.t. β and set it to zero

$$\frac{\partial}{\partial \beta} E_{\text{ML}}(\boldsymbol{w}_{\text{ML}}, \beta) = \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}_{\text{ML}}^{T} \boldsymbol{\phi}(\boldsymbol{x}_{i}) - y_{i})^{2} - \frac{N}{2\beta} \stackrel{!}{=} 0 \qquad (45)$$

Solving for β

$$\frac{1}{\beta_{\text{ML}}} = \frac{1}{N} \sum_{i=1}^{N} (\boldsymbol{w}_{\text{ML}}^{T} \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2$$
(46)

Predicting for new data

$$y \sim \mathcal{N}(f_{\boldsymbol{w}}(\boldsymbol{x}), \beta^{-1}) \tag{47}$$

Plugging in the $w_{\rm ML}$ and $\beta_{\rm ML}$ into our likelihood we get a predictive distribution that allows us to make prediction \hat{y}_{new} for the new data x_{new} .

$$p(\hat{y}_{new} \mid \boldsymbol{x}_{new}, \boldsymbol{w}_{\text{ML}}, \beta_{\text{ML}}) = \mathcal{N}(\hat{y}_{new} \mid \boldsymbol{w}_{\text{ML}}^T \boldsymbol{\phi}(\boldsymbol{x}_{new}), \beta_{\text{ML}}^{-1})$$
 (48)

Posterior distribution

Recall from the Lecture 3, that ML leads to overfitting (especially, when little training data is available).

Solution - consider the posterior distribution instead

$$p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \beta, \cdot) = \underbrace{\frac{p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \cdot p(\boldsymbol{w} \mid \cdot)}{p(\boldsymbol{X}, \boldsymbol{y})}}_{\text{normalizing constant}}$$
(49)

$$\propto p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \cdot p(\boldsymbol{w} \mid \cdot)$$
 (50)

Linear Regression 39

Precision $\beta = 1/\sigma^2$ is treated as a known parameter to simplify the calculations.

Posterior distribution

Recall from the Lecture 3, that ML leads to overfitting (especially, when little training data is available).

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$$p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \beta, \cdot) = \underbrace{\frac{p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \cdot p(\boldsymbol{w} \mid \cdot)}{p(\boldsymbol{X}, \boldsymbol{y})} \cdot p(\boldsymbol{w} \mid \cdot)}_{\text{normalizing constant}}$$

$$(49)$$

$$\propto p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) \cdot p(\boldsymbol{w} \mid \cdot)$$
 (50)

Connection to the coin flip example

	train data	likelihood	prior	posterior
coin:	$\mathcal{D} = X$	$p(\mathcal{D} \mid \theta)$	$p(\theta \mid a, b)$	$p(\theta \mid \mathcal{D})$
regr.:	$\mathcal{D} = \{oldsymbol{X}, oldsymbol{y}\}$	$p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta)$	$p(\boldsymbol{w} \mid \cdot)$	$p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \beta, \cdot)$

How do we choose the prior $p(\boldsymbol{w} \mid \cdot)$?

Precision $\beta = 1/\sigma^2$ is treated as a known parameter to simplify the calculations.

Prior for $oldsymbol{w}$

We set the prior over $oldsymbol{w}$ to an isotropic multivariate normal distribution with zero mean

$$p(\boldsymbol{w} \mid \alpha) = \mathcal{N}(\boldsymbol{w} \mid \boldsymbol{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \exp\left(-\frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w}\right)$$
 (51)

where,

 α - precision of the distribution

41

M - number of elements in the vector ${m w}$

Motivation:

- Higher probability is assigned to small values of w
 prevents overfitting (recall slide 21)
- Likelihood is also Gaussian simplified calculations

Linear Regression

Maximum a posteriori (MAP)

We are looking for $oldsymbol{w}$ that corresponds to the mode of the posterior

$$\mathbf{w}_{\text{MAP}} = \underset{\mathbf{w}}{\text{arg max}} \ p(\mathbf{w} \mid \mathbf{X}, \mathbf{y}, \alpha, \beta)$$
 (52)

$$= \underset{\boldsymbol{w}}{\operatorname{arg \, max}} \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) + \ln p(\boldsymbol{w} \mid \alpha) - \underbrace{\ln p(\boldsymbol{X}, \boldsymbol{y})}_{=\operatorname{const}}$$
(53)

$$= \underset{\boldsymbol{w}}{\operatorname{arg\,min}} - \ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) - \ln p(\boldsymbol{w} \mid \alpha)$$
 (54)

Similar to ML, define the MAP error function as negative log-posterior

$$E_{\text{MAP}}(\boldsymbol{w}) = -\ln p(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}, \alpha, \beta)$$
(55)

$$= -\ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \beta) - \ln p(\boldsymbol{w} \mid \alpha) + \text{const}$$
 (56)

We ignore the constant terms in the error function, as they are independent of $oldsymbol{w}$

Data Mining and Analytics

MAP error function

Simplify the error function

$$\begin{split} E_{MAP} &= -\ln p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{w}, \boldsymbol{\beta}) - \ln p(\boldsymbol{w} \mid \boldsymbol{\alpha}) \\ &= \frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 - \frac{N}{2} \ln \boldsymbol{\beta} + \frac{N}{2} \ln 2\pi \\ &- \ln \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} + \frac{\alpha}{2} \boldsymbol{w}^T \boldsymbol{w} \\ &= \frac{\beta}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 + \frac{\alpha}{2} \|\boldsymbol{w}\|_2^2 + \text{ const} \\ &= \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i) - y_i)^2 + \frac{\lambda}{2} \|\boldsymbol{w}\|_2^2 + \text{ const} \qquad \text{where } \lambda = \frac{\alpha}{\beta} \\ &\xrightarrow{\text{ridge regression error fn!}} \\ &= E_{\text{ridge}}(\boldsymbol{w}) + \text{const} \end{split}$$

MAP estimation with Gaussian prior is equivalent to ridge regression!

(57)

Predicting for new data

Recall, that

$$y \sim \mathcal{N}(f_{\boldsymbol{w}}(\boldsymbol{x}), \beta^{-1})$$
 (58)

Plugging in the $w_{\rm MAP}$ into our likelihood we get a predictive distribution that lets us make prediction \hat{y}_{new} for the new data x_{new} .

$$p(\hat{y}_{new} \mid \boldsymbol{x}_{new}, \boldsymbol{w}_{MAP}, \beta) = \mathcal{N}(\hat{y}_{new} \mid \boldsymbol{w}_{MAP}^T \boldsymbol{\phi}(\boldsymbol{x}_{new}), \beta^{-1})$$
 (59)

Recall, that we assume β to be known a priori (for simplified calculations).