Introduction to Machine Learning

Chap II: Regression



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Outline

Linear regression

- Basic concepts
- Non linear data and basis functions

Model optimization

- How to control your model
- How to optimize your model

Model minimization

Gradient descent

Bonus: Likelihood and regression (*)

Notations

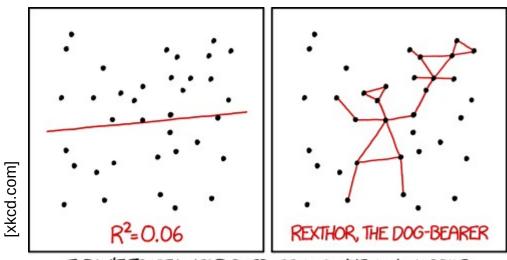
• Variable/feature: x, weight: w

• Vector: variables
$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$
; weights $\mathbf{w} = \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}$

- Vector (transpose): $\mathbf{x}^T = (x_1, \dots, x_n)$
- Dot product: $\mathbf{w} \cdot \mathbf{x} = \mathbf{w}^T \mathbf{x} = \sum_{i=1}^n w_i x_i = w_1 x_1 + w_2 x_2 + \dots + w_n x_n$.
- Sequence of p vectors: $\{\mathbf{x}_j\}_{(j=1..p)}$

• Matrix (size
$$n \times m$$
): $\mathbf{M} = \begin{pmatrix} a_{11} & \cdots & a_{1m} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nm} \end{pmatrix}$

Linear regression



I DON'T TRUST LINEAR REGRESSIONS WHEN IT'S HARDER TO GUESS THE DIRECTION OF THE CORRELATION FROM THE SCATTER PLOT THAN TO FIND NEW CONSTELLATIONS ON IT.

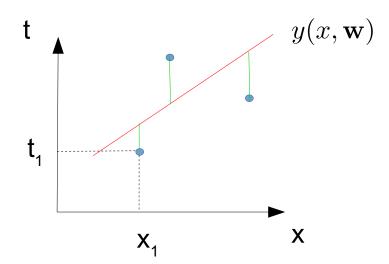
Simple case: 1 dimensional data

Training dataset

- N observations of **feature** $x = \{x_1, ..., x_N\}$
- N Target values $t = \{t_1, ..., t_N\}$

Prediction model: straight line

$$y(x, \mathbf{w}) = y(x; w_0, w_1) = w_0 + w_1 x$$



Weights determined by minimizing an Error function E

 also called Cost function or Loss function (i.e what is the consequence of your error!)

Common choice: sum of **square distance** between function and target:

$$E(w_0, w_1) = \sum_{i=1}^{N} \{y(x_i; w_0, w_1) - t_i\}^2$$

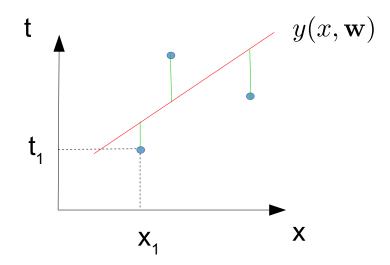
Simple case: 1 dimensional data

Training dataset

- N observations of **feature** $x = \{x_1, ..., x_N\}$
- N Target values $t = \{t_1, ..., t_N\}$

Prediction model: straight line

$$y(x, \mathbf{w}) = y(x; w_0, w_1) = w_0 + w_1 x$$



Here optimal weights can be calculated analytically (not always possible!)

$$E(w_0, w_1) = \sum_{i=1}^{N} \{y(x_i; w_0, w_1) - t_i\}^2$$

$$\begin{cases} \frac{\partial E(w_0, w_1)}{\partial w_0} = 0 \\ \frac{\partial E(w_0, w_1)}{\partial w_1} = 0 \end{cases} \Leftrightarrow \begin{cases} w_1 = \frac{\text{cov}(x, t)}{\text{var}(x)} = r \frac{\sigma(t)}{\sigma(x)} \\ w_0 = \bar{t} - r \frac{\sigma(t)}{\sigma(x)} \bar{x} \end{cases}$$

(r: correlation factor between x and t)

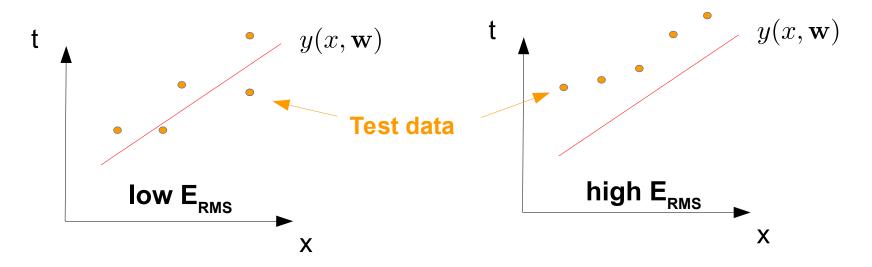
Simple case: 1 dimensional data

Training and testing

- Training: use dataset to determine weights w₀ and w₁
- **Testing**: check compatibility of $y(x, \mathbf{w})$ on a new dataset

Measure of **compatibility**: root mean squared error (RMS)

$$E_{RMS} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \{y(x_i, \mathbf{w}) - t_i\}^2} = \sqrt{\frac{E(\mathbf{w})}{N}}$$



Generalization: multidimensional data

Dataset (p x 1 data)

N observations of p-dimensions features

$$\{\mathbf{x_i}\}_{i=1..N} = \{\mathbb{R}^p\} = \left\{ \begin{pmatrix} x_1 \\ \vdots \\ x_p \end{pmatrix} \right\}$$

N target values t = {t₁, ..., t_N}

$y(\mathbf{x}, \mathbf{w})$ \mathbf{x}_{1} 2D example

Fit function: multidimensional plane

Linear function with p+1 weights: w

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \mathbf{w}^T \mathbf{x} = w_0 + w_1 x_1 + w_2 x_2 + \dots w_p x_p.$$
bias term

Generalization: multidimensional data

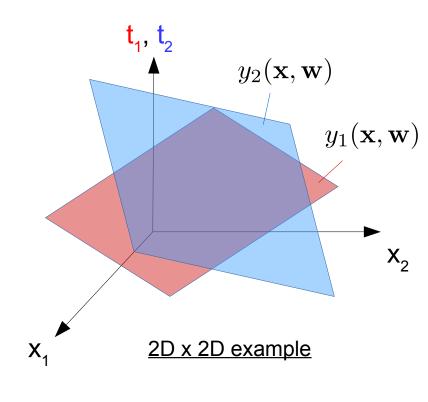
Dataset (p x q data)

N observations of p-dimensions features

$$\{\mathbf{x_i}\}_{i=1..N} = \{\mathbb{R}^p\} = \left\{ \begin{pmatrix} x_1 \\ \vdots \\ x_p \end{pmatrix} \right\}$$

N target values of q-dimensions

$$\{\mathbf{t_i}\}_{i=1..N} = \{\mathbb{R}^q\} = \left\{ \left(\begin{array}{c} t_1 \\ \vdots \\ t_q \end{array}\right) \right\}$$

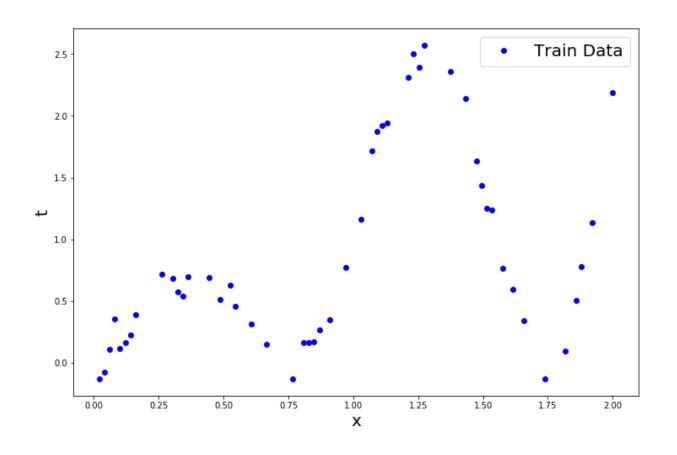


Fit functions:

$$\begin{pmatrix} y_1(\mathbf{x}, \mathbf{w}) \\ \vdots \\ y_q(\mathbf{x}, \mathbf{w}) \end{pmatrix} = \begin{pmatrix} w_{01} \\ \vdots \\ w_{0q} \end{pmatrix} + \begin{pmatrix} w_{11} & \cdots & w_{1p} \\ \vdots & \ddots & \vdots \\ w_{q1} & \cdots & w_{qp} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_p \end{pmatrix}$$

bias terms

What if your data is not linear?



→ use basis functions

Apply M non-linear basis functions ϕ to input feature x:

$$\mathbf{x} \longrightarrow \left(egin{array}{c} \phi_1(\mathbf{x}) \ dots \ \phi_M(\mathbf{x}) \end{array}
ight) \qquad \phi_j(\mathbf{x}) : ext{ basis function}$$

The regression function y(x, w) then become non-linear function of x:

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{i=1}^{M} w_i \phi_i(\mathbf{x}) = w_0 + w_1 \phi_1(\mathbf{x}) + \dots + w_M \phi_M(\mathbf{x})$$

These functions are called linear models because they are linear in w.

For high number of dimensions linear models suffer from **limitations**, and other approaches (as Neural Networks) are more suited.

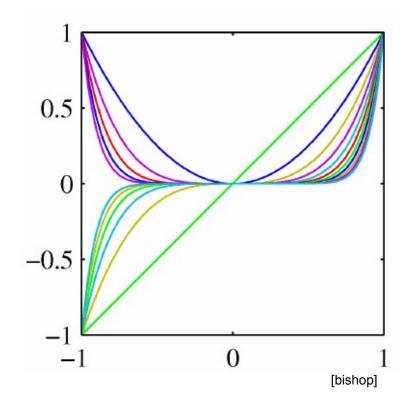
Polynomial basis functions (1D)

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

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

Global functions of input variable

→ a small change in x affects all
basis functions



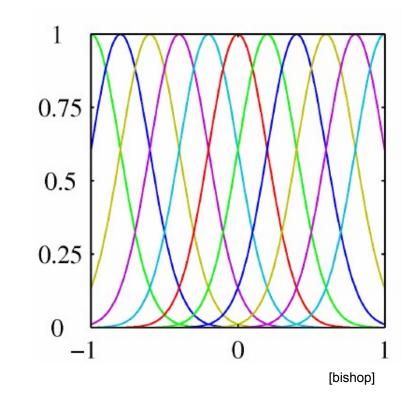
Gaussian basis functions (1D)

$$\phi_j(x) = e^{-\frac{(x-\mu_j)^2}{2\sigma^2}}$$
$$y(x, \mathbf{w}) = \sum_{j=0}^{M-1} w_j e^{-\frac{(x-\mu_j)^2}{2\sigma^2}}$$

Parameters:

 μ_{j} (location) and σ (width) Normalization is not relevant.

local functions of input variable
 → a small change in x mostly
 affects nearby basis functions



Sigmoidal basis functions (1D)

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

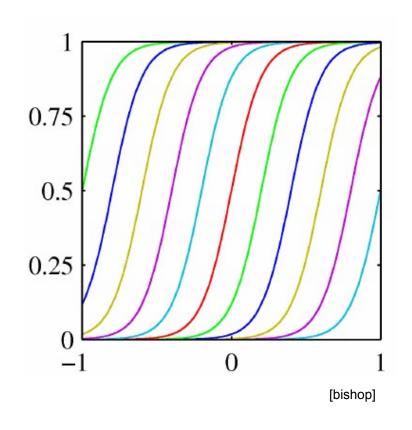
with

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

Parameters:

 μ_i (location) and s (slope)

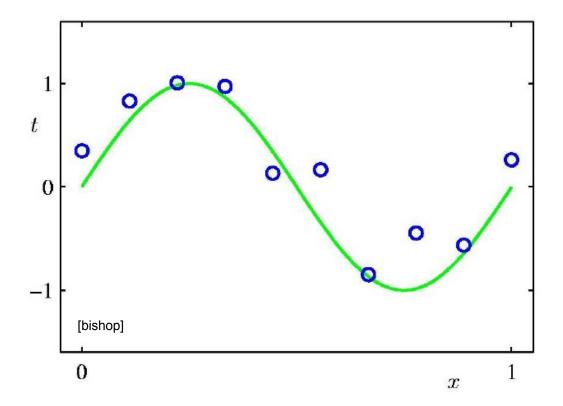
local functions of input variable
 → a small change in x mostly
 affects nearby basis functions



Example: polynomial curve fitting

Training dataset

- N observations of $x = \{x_1, ..., x_N\}$: uniformly spaced in [0,1]
- Target values $t = \{t_1, ..., t_N\}$: $sin(2\pi x) + Gaussian noise$



Dummy example but could be e.g. temperature (t) evolution over 1 day (x)

Polynomial curve fitting

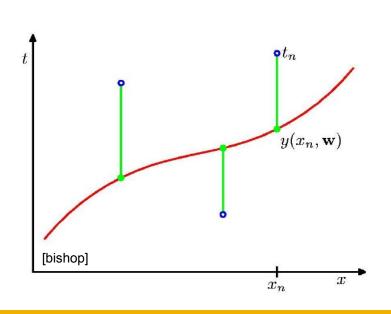
Fit function

• Polynomial function of degree **M**, with coefficients $\mathbf{w} = (w_1, ..., w_M)^T$

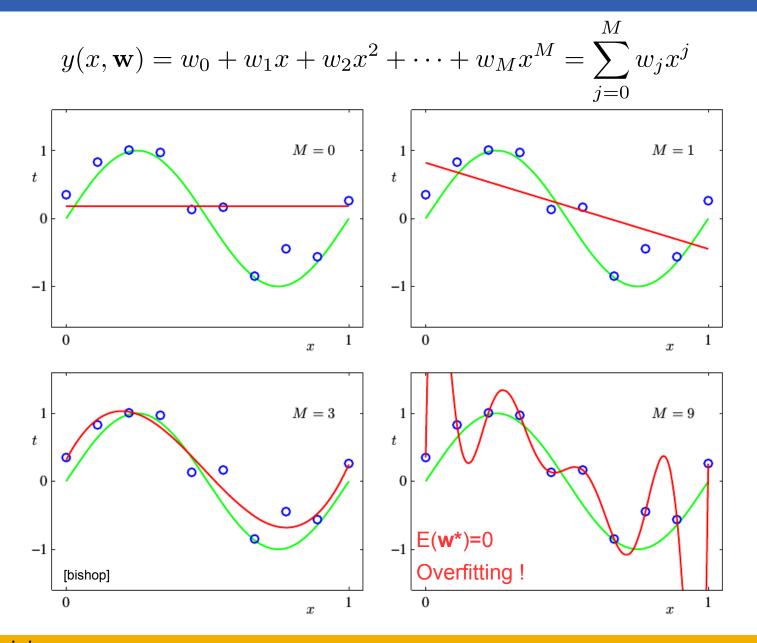
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \dots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

- Non-linear function of x, but linear function of $\mathbf{w} \to \mathbf{linear} \ \mathbf{model}$
- Values of coefficient obtained by minimizing an error function
- Sum of the square of the errors E(w)

$$E(\mathbf{w}) = \sum_{i=1}^{N} \left\{ y(x_i, \mathbf{w}) - t_i \right\}^2$$
 Minimization Fitted weights \mathbf{w}^* $\mathbf{E}(\mathbf{w}^*)$





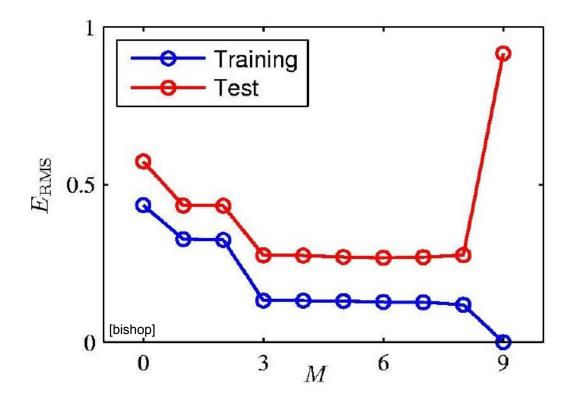


It is instructive to look at the **fitted weights** for various cases: when M increases the coefficient become **fine tuned** to data by developing large positive and negative values.

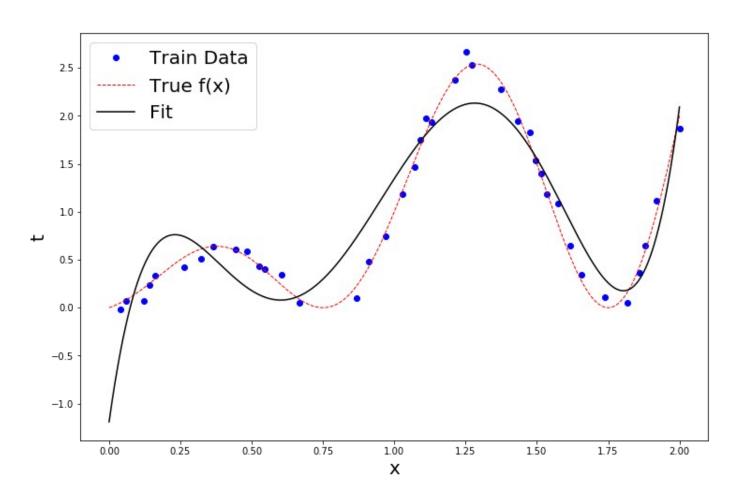
	M=0	M = 1	M = 3	M = 9
w_0^{\star}	0.19	0.82	0.31	0.35
w_1^\star		-1.27	7.99	232.37
w_2^\star			-25.43	-5321.83
w_3^{\star}			17.37	48568.31
w_4^{\star}				-231639.30
w_5^{\star}				640042.26
w_6^{\star}				-1061800.52
w_7^{\star}				1042400.18
w_8^{\star}				-557682.99
w_9^{\star}				125201.43

Root mean squared error (RMS)

$$E_{RMS} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \{y(x_i, \mathbf{w}) - t_i\}^2} = \sqrt{\frac{E(\mathbf{w})}{N}}$$



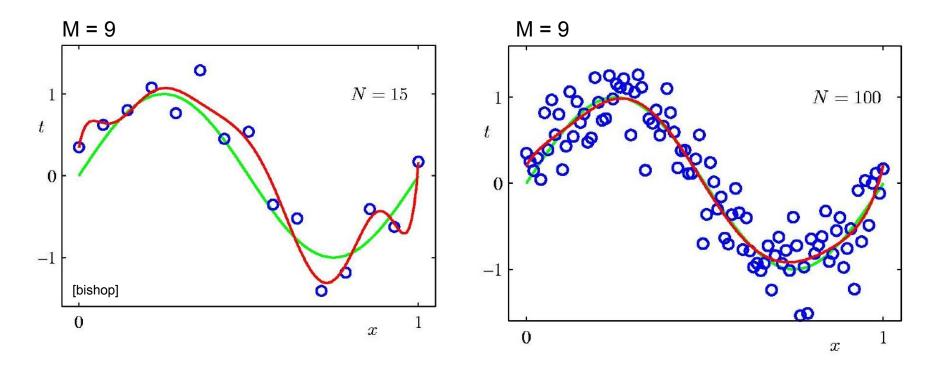
What if your model completely fails?



→ try to regularize your model

Regularization

Overfitting really depends on **N** data and **M** parameters.



How can we constrain the fitted parameter into reasonable values?

→ **Regularization** techniques can be a solution.

Regularization

Add **penalization term** to error function in order to **constrain** parameters **w**.

→ Simple penalization: **ridge regression** (L2 norm) Constrains weight to be not too large.

$$\tilde{E}(\mathbf{w}) = \sum_{i=1}^{N} \left\{ y(x_i, \mathbf{w}) - t_i \right\}^2 + \lambda ||\mathbf{w}||^2$$
where $||\mathbf{w}||^2 = \mathbf{w}^T \mathbf{w} = w_0^2 + \dots + w_M^2$

where
$$||\mathbf{w}||^2 = \mathbf{w^T}\mathbf{w} = w_0^2 + \dots + w_M^2$$

and λ : parameter that governs the importance of regularization

Other choices

- Lasso regression (L1 norm): $||\mathbf{w}|| = |w_0| + ... + |w_M|$ Reduce number of weights (set some of them to 0)
- Elastic net: L1 + L2 norm

Regularization (*)

General regularization term is of the form:

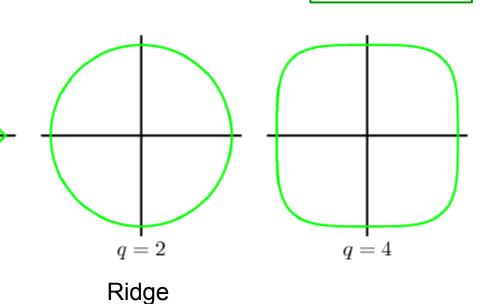
$$\tilde{E}(\mathbf{w}) = \sum_{i=1}^{N} \{y(x_i, \mathbf{w}) - t_i\}^2 + \lambda \sum_{j=1}^{M} |w_j|^q$$

Minimizing this error function is equivalent to minimizing the unregularized sum-of-square error with the constraint

q=1

Lasso

(L1 norm)



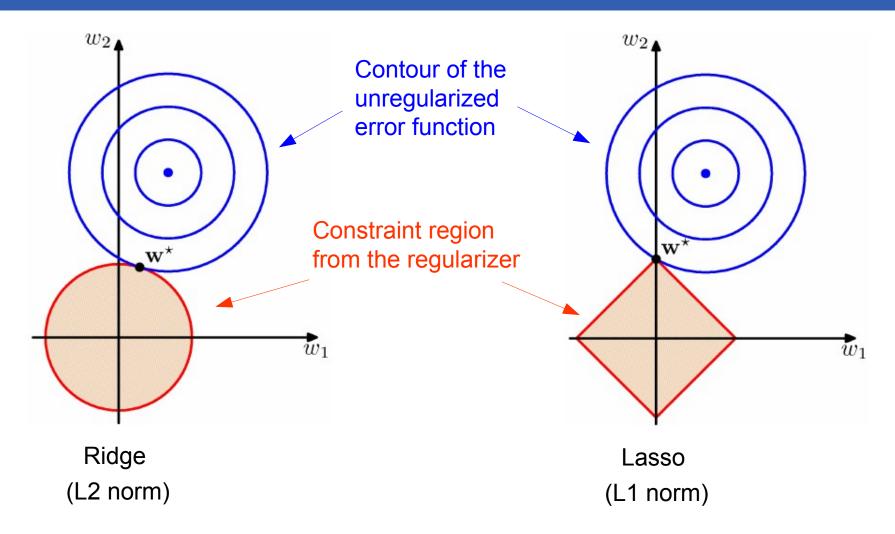
(L2 norm)

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q = 0.5

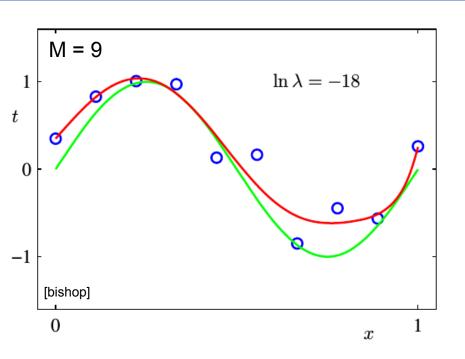
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Regularization (*)



The optimum value for the parameter vector w is denoted by w^{*}. The lasso gives a sparse solution in which $w_1^* = 0$.

Regularization



$\int_{t}^{1} M = 9$	$\ln \lambda = 0$	-
0	0 0	°
-1		9
0		x 1

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
w_0^{\star}	0.35	0.35	0.13
w_1^{\star}	232.37	4.74	-0.05
w_2^{\star}	-5321.83	-0.77	-0.06
w_3^{\star}	48568.31	-31.97	-0.05
w_4^{\star}	-231639.30	-3.89	-0.03
w_5^{\star}	640042.26	55.28	-0.02
w_6^{\star}	-1061800.52	41.32	-0.01
w_7^{\star}	1042400.18	-45.95	-0.00
w_8^{\star}	-557682.99	-91.53	0.00
w_9^\star	125201.43	72.68	0.01

Effect of L2 norm regularization

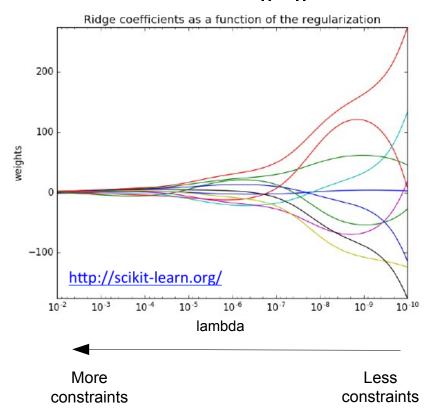
• In λ = -inf : no regularization

• In $\lambda = -18$: suppressed overfitting

• In λ = 0: fit too constrained

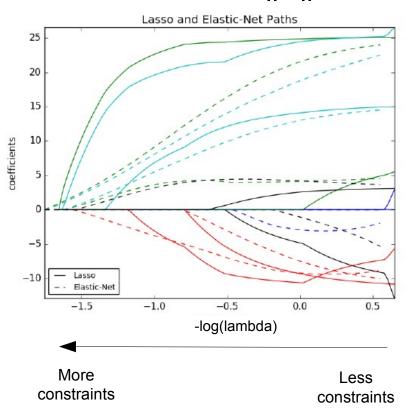
Regularization

L2 norm: $\lambda ||\mathbf{w}||^2$



Affects value of coefficients (shrinkage)

L1 norm: $\lambda ||\mathbf{w}||$



Affects number of coefficients (sparsity)

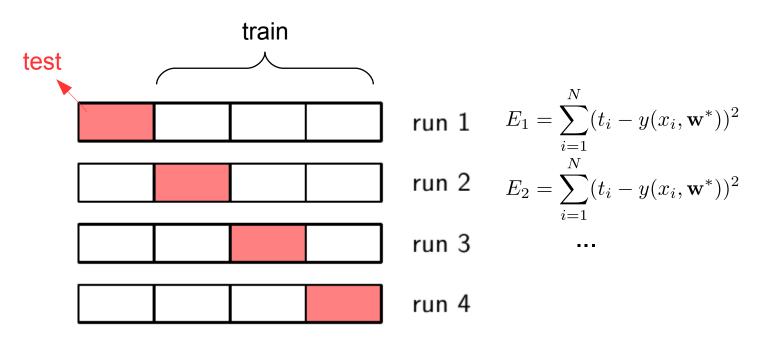
Model selection



Model selection

K-fold cross-validation

Divide data in K groups, use K-1 for training and test on left-over group Rinse and repeat K times



Cross-validation error: $CV = \frac{1}{K} \sum E_i$

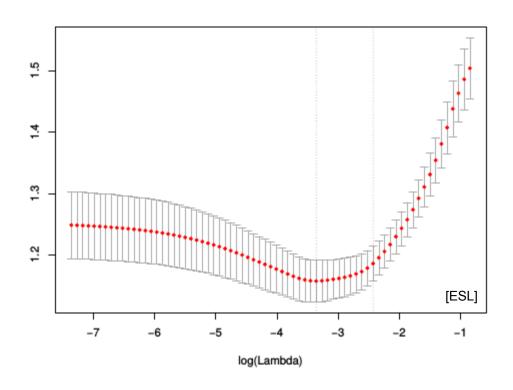
Choose the set of hyper-parameters (ex λ) that give the smallest CV.

Drawback: can be very time consuming ...

Model selection

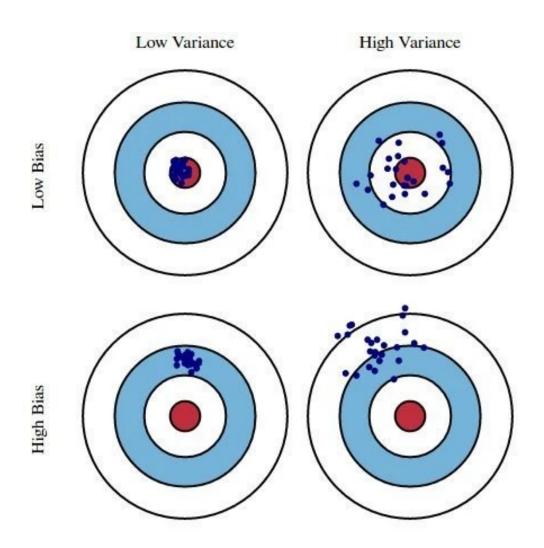
K-fold cross-validation

Divide data in K groups, use K-1 for training and test on left-over group Rinse and repeat K times



Cross-validation curve

What is a good model?



[figure: kdnuggets.com]

The Bias-Variance decomposition

Noise

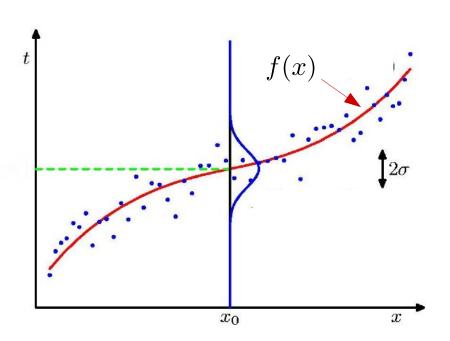
(Mean 0,

variance σ^2)

Training dataset

- N observations of **feature** $x = \{x_1, ..., x_N\}$
- N Target values $t = \{t_1, ..., t_N\}$

We assume that **t** are distributed following a function: $t_i = f(x_i) + \epsilon$



 \rightarrow We want to find y(x) that approximates true function f(x)

The Bias-Variance decomposition (*)

As before we determine y(x) by minimizing: $\sum_{i=1}^{N} \{y(x_i, \mathbf{w}) - t_i\}^2$ over the **training** dataset

The **expected error** for a **new test sample x** can be decomposed as:

- Data noise: minimal error of the model
- Bias in the model: error caused by model assumptions
- Variance of model: how much y(x) depends on structure of data

The Bias-Variance decomposition (*)

As before we determine y(x) by **minimizing**: $\sum \left\{y(x_i,\mathbf{w})-t_i\right\}^2$ over the **training** dataset

$$\sum_{i=1}^{N} \left\{ y(x_i, \mathbf{w}) - t_i \right\}^2$$

The **expected error** for a **new test sample x** can be decomposed as:

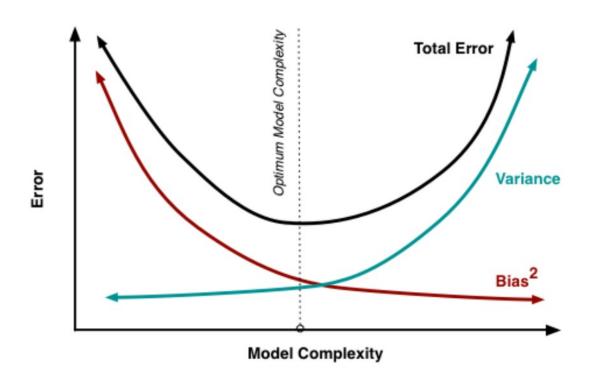
- Data noise: minimal error of the model
- Bias in the model: error caused by model assumptions
- Variance of model: how much y(x) depends on structure of data

Mean squared error:

$$\mathbb{E}[(y(x) - f(x))^2] = \sigma^2 + (\mathbb{E}[y(x)] - f(x))^2 + \mathbb{E}[(y(x) - \mathbb{E}[y(x)])^2]$$

The expectation \mathbb{E} is calculated over different choices of the training dataset

The Bias-Variance decomposition



Simple models **under-fit**: deviate from data (high bias) but not influenced by structure of data (low variance)

Complex models **over-fit**: small deviation from data (low bias) but very sensitive to data fluctuations (high variance)

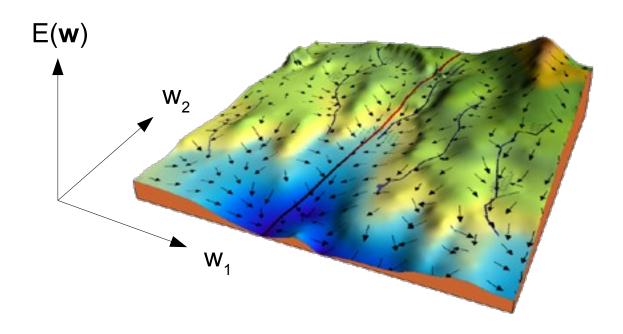
Gradient descent



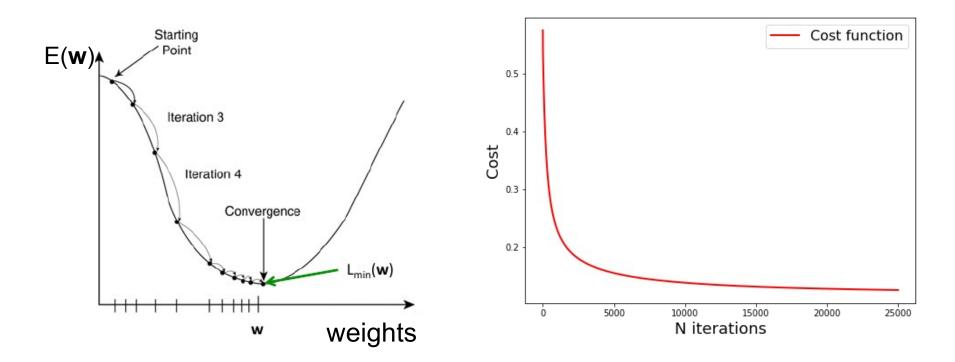
How can we **minimize** the error function for complex cases (ex: when there is no analytic solution)?

→ Solution: Gradient descent

Iteratively move in the direction of steepest descent as defined by the negative of the gradient of the error function



Descend along the error function to find a (local) minimum:



Direction of descent:

→ (negative of the **gradient** of the error function) × (**learning rate**)

Example: fit N data points with linear function: $y(x, \mathbf{w}) = w_0 + w_1 x$

Error function and its derivatives

$$E(w_0, w_1) = \sum_{i=1}^{N} \{y(x_i, \mathbf{w}) - t_i\}^2 = \sum_{i=1}^{N} \{(w_0 + w_1 x_i) - t_i\}^2$$

$$\left\{ \frac{\partial E(w_0, w_1)}{\partial w_0} = \sum_{i=1}^{N} 2\{(w_0 + w_1 x_i) - t_i\} \right\}$$

$$\frac{\partial E(w_0, w_1)}{\partial w_1} = \sum_{i=1}^{N} 2x_i \{(w_0 + w_1 x_i) - t_i\}$$

Example: fit N data points with linear function: $y(x, \mathbf{w}) = w_0 + w_1 x$

Error function and its derivatives

$$E(w_0, w_1) = \sum_{i=1}^{N} \{y(x_i, \mathbf{w}) - t_i\}^2 = \sum_{i=1}^{N} \{(w_0 + w_1 x_i) - t_i\}^2$$

$$\longrightarrow \begin{cases} \frac{\partial E(w_0, w_1)}{\partial w_0} = \sum_{i=1}^{N} 2\{(w_0 + w_1 x_i) - t_i\} \\ \frac{\partial E(w_0, w_1)}{\partial w_1} = \sum_{i=1}^{N} 2x_i \{(w_0 + w_1 x_i) - t_i\} \end{cases}$$

Iterative update **rule**:

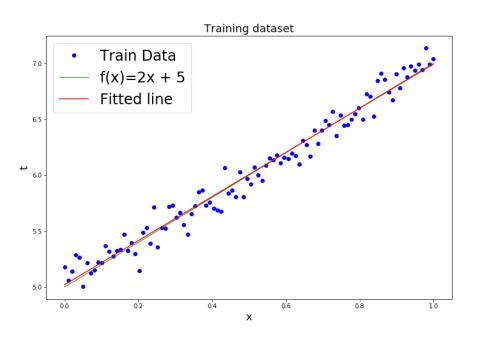
$$\begin{aligned} \mathbf{w}_0^{(k)} &\to w_0^{(k+1)} = w_0^{(k)} - \frac{\partial E(w_0, w_1)}{\partial w_0} \times \eta \\ \mathbf{w}_1^{(k)} &\to w_1^{(k+1)} = w_1^{(k)} - \frac{\partial E(w_0, w_1)}{\partial w_1} \times \eta \end{aligned} \quad \text{k: iteration num}$$

$$\mathbf{\eta: learning rate}$$

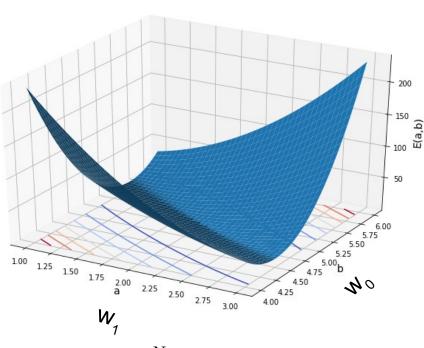
k: iteration number

Repeat until convergence

Input data: $\{x_i, t_i\}$

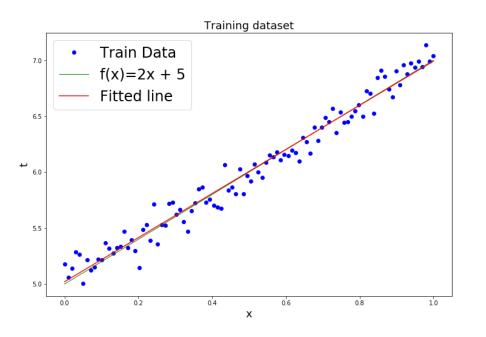


Error function

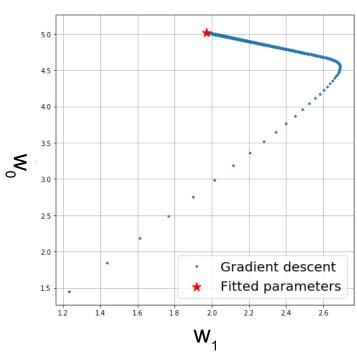


$$E(w_0, w_1) = \sum_{i=1}^{N} \{(w_0 + w_1 x_i) - t_i\}^2$$

Input data: $\{x_i, t_i\}$



Gradient descent



$$\mathbf{w}_0^{(k)} \to \mathbf{w}_0^{(k+1)} = \mathbf{w}_0^{(k)} - \frac{\partial E(\mathbf{w}_0, \mathbf{w}_1)}{\partial \mathbf{w}_0} \times \eta$$

$$\mathbf{w}_{1}^{(k)} \to \mathbf{w}_{1}^{(k+1)} = \mathbf{w}_{1}^{(k)} - \frac{\partial E(\mathbf{w}_{0}, \mathbf{w}_{1})}{\partial \mathbf{w}_{1}} \times \eta$$

1000 iterations learning rate $\eta = 0.05$

Stochastic gradient descent

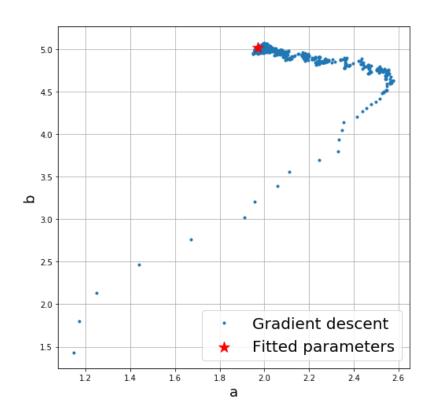
Gradient descent can be **computationally costly** for large N since the gradient is calculated over full training set.

→ Solution: Stochastic gradient descent

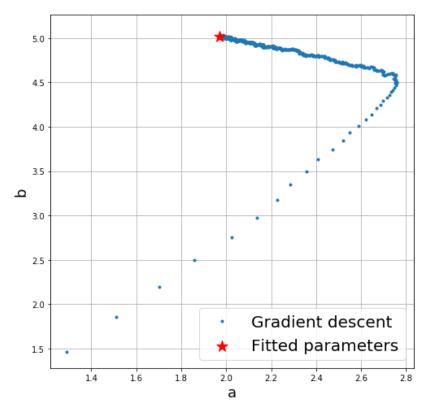
Compute gradient on a small **batch** of events (can be 1 event):

$$\begin{cases} \frac{\partial E(w_0, w_1)}{\partial w_0} = \sum_{i \subset N} 2 \left\{ (w_0 + w_1 x_i) - t_i \right\} \\ \frac{\partial E(w_0, w_1)}{\partial w_1} = \sum_{i \subset N} 2x_i \left\{ (w_0 + w_1 x_i) - t_i \right\} \end{cases}$$

Stochastic gradient descent



Gradient calculated on 1 (random) event at each step



Gradient calculated on 10 (random) events at each step

Going further (*)



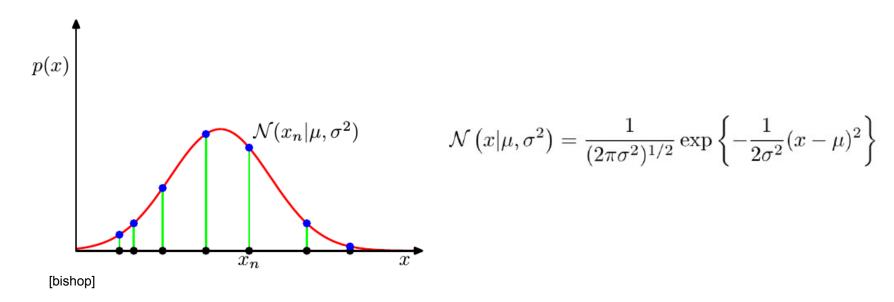
Likelihood

Consider N measurements of x distributed along a given probability law p(x).

$$\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$$

where values x_i are **independent and identically distributed** (i.i.d).

Ex: Normal (a.k.a Gaussian) law with 2 parameters: mean μ and variance σ²



What is the *likelihood* of this set of measurements? Can we estimate μ and σ given \mathbf{x} ?

Likelihood and parameter estimation

Since the variables x are i.i.d we can write the joint probability distribution, therefore the **likelihood** of the dataset, given μ and σ is:

$$\mathcal{L}(\mu, \sigma^2; \mathbf{x}) \equiv p(\mathbf{x}|\mu, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(x_n|\mu, \sigma^2)$$

To **estimate** μ and σ given **x** one **maximizes** p w.r.t these parameters. In practice often maximize $\ln(p)$ or minimize $-\ln(p)$.

$$\ln p(\mathbf{x}|\mu,\sigma^2) = -\frac{1}{2\sigma^2} \sum_{m=1}^{N} (x_n - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi)$$

$$\begin{cases} \frac{\partial(\ln p(\mathbf{x}|\mu, \sigma^2))}{\partial \mu} = 0 \to \mu_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} x_n \\ \frac{\partial(\ln p(\mathbf{x}|\mu, \sigma^2))}{\partial \sigma} = 0 \to \sigma_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\mathrm{ML}})^2 \end{cases}$$

Expected values

$$\mathbb{E}[\mu_{\mathrm{ML}}] = \mu$$

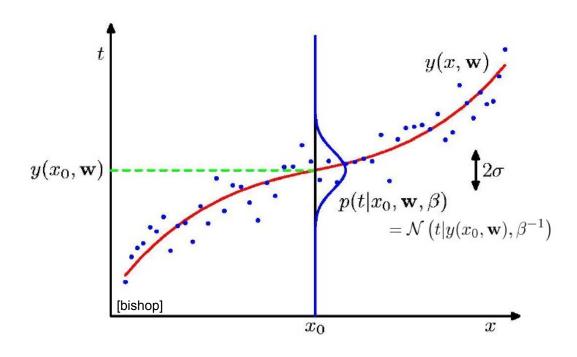
$$\mathbb{E}[\sigma_{\mathrm{ML}}^2] = \left(\frac{N-1}{N}\right)\sigma^2$$

Curve fitting with noise

Assume target variable in training dataset is subject to Gaussian noise

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

where $\beta = \frac{1}{\sigma^2}$ is a precision parameter.



Predictive probabilistic model

By maximizing the likelihood on the training dataset we obtain a probabilistic predictive model for *t* (instead of a single point estimate):

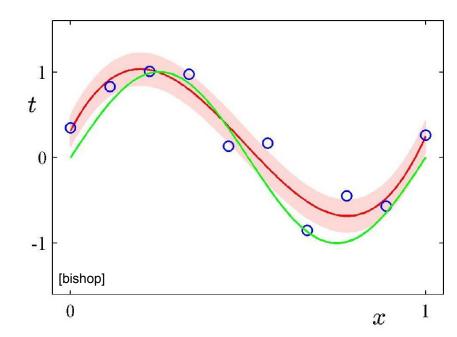
$$p(t|x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}\left(t|y(x, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1}\right)$$

where \mathbf{w}_{MI} is obtained by minimizing the sum of square error $E(\mathbf{w})$

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$

and β_{MI} is given by

$$\frac{1}{\beta_{\text{ML}}} = \frac{1}{N} \sum_{n=1}^{N} \left\{ y(x_n, \mathbf{w}_{\text{ML}}) - t_n \right\}^2$$



Exercice: show this!

Hints →

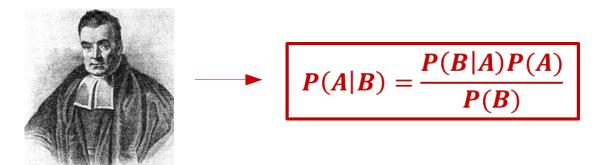
$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|y(x_n, \mathbf{w}), \beta^{-1})$$

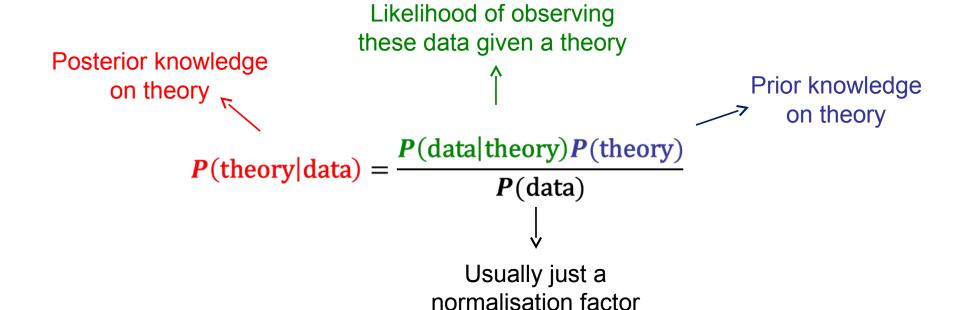
$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\underbrace{\frac{\beta}{2} \sum_{n=1}^{N} \left\{ y(x_n, \mathbf{w}) - t_n \right\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)}_{\beta E(\mathbf{w})}$$

 \mathbf{w}_{MI} is determined by minimizing sum of square error $E(\mathbf{w})$, then:

$$\frac{1}{\beta_{\text{ML}}} = \frac{1}{N} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}_{\text{ML}}) - t_n\}^2$$

Bayes theorem and likelihood





Bayesian approach

We assume that unknown parameters **w** follow a Gaussian *prior* of the form:

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

According to **Bayes Theorem** we have the *posterior*:

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

Taking $-ln(p) \rightarrow$ the maximum of the posterior is given by the minimum of:

$$\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \boxed{\frac{\alpha}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}}$$
 Regularization parameter with $\lambda = \alpha/\beta$