# COMPUTATIONAL STATISTICS LINEAR REGRESSION

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## OUTLINE







- Consider training data (x<sub>n</sub>, y<sub>n</sub>)<sub>n=1,...,N</sub>. We want to find the best linear fit to this data, i.e. the best straight line y(x) = w<sub>1</sub> · x + w<sub>0</sub>
- Let's take a curve fitting approach, and find the coefficients  $\mathbf{w} = (w_0, w_1)$  that minimise sum-of-squares error

$$E(\mathbf{w}) = \sum_{n=1}^{N} [y_n - y(x_n)]^2$$

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Ν	W <sub>0</sub>	<i>W</i> <sub>1</sub>	
5	5.3812	8.1856	
10	2.9735	9.6608	
20	3.5493	9.6204	
50	3.2084	9.9253	
100	2.8327	9.8894	
1000	3.0451	9.9464	
10000	2.9937	10.0147	
100000	3.0084	9.9992	

## **GENERALISED BASIS FUNCTIONS**

- Suppose our inputs are real vectors, and outputs are real numbers, and we have observations (x<sub>i</sub>, y<sub>i</sub>), i = 1,..., N.
- We consider a set of *M* basis functions φ<sub>j</sub> : ℝ<sup>n</sup> → ℝ, and write φ(**x**) = (φ<sub>0</sub>(**x**),...,φ<sub>M-1</sub>(**x**)). By convention, φ<sub>0</sub> ≡ 1.
- We consider the linear model

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

 y(x, w) is linear in the parameters w, but can be non-linear in the input state x.

## **GENERALISED BASIS FUNCTIONS**

Basis functions can, and usually are, non-linear functions of the inputs. Examples are

- Polynomials up to degree d. In 1 dimension,  $1, x, x^2, \ldots, x^d$
- Gaussian basis functions:  $\phi_j = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$ , where  $\mu_j$  is the location and *s* is the lengthscale of the Gaussian.

• Sigmoid functions 
$$\phi_j = \sigma\left(rac{x-\mu_j}{s}
ight)$$
, with  $\sigma(a) = rac{1}{1+\exp(-a)}$ 



Figure 3.1 Examples of basis functions, showing polynomials on the left, Gaussians of the form (3.4) in the centre, and sigmoidal of the form (3.5) on the right.

- Assume Gaussian noise:  $t = y(\mathbf{x}, \mathbf{w}) + \epsilon, \epsilon \sim \mathcal{N}(0, \beta^{-1})$
- Hence  $p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(y(\mathbf{x}, \mathbf{w}), \beta^{-1})$

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- Given observations **X**, **t**:  $(\mathbf{x}_i, t_i)_{i=1,...,N}$ , the likelihood is then

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{i=1}^{N} \mathcal{N}(y_i | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i), \beta^{-1})$$

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giving a log likelihood of

$$\ln p(\mathbf{t}|\mathbf{w},\beta) = \sum_{n=1}^{N} \ln \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1})$$
$$= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w})$$
(3.11)

where the sum-of-squares error function is defined by

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\}^2.$$
 (3.12)

• Compute the gradient w.r.t. **w** of the log-likelihood, set it to zero and solve for **w**.

 Compute the gradient w.r.t. w of the log-likelihood, set it to zero and solve for w.

$$\mathbf{w}_{\mathrm{ML}} = \left(\mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}$$
(3.15)

which are known as the *normal equations* for the least squares problem. Here  $\Phi$  is an  $N \times M$  matrix, called the *design matrix*, whose elements are given by  $\Phi_{nj} = \phi_j(\mathbf{x}_n)$ , so that

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}.$$
(3.16)

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Looking for the ML solution of the precision β, we get

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N} \sum_{n=1}^{N} \{t_n - \mathbf{w}_{\mathrm{ML}}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\}^2$$
(3.21)

#### MAXIMUM LIKELIHOOD REGRESSION: BIAS TERM

• The parameter  $w_0$  is known also as bias term.

At this point, we can gain some insight into the role of the bias parameter  $w_0$ . If we make the bias parameter explicit, then the error function (3.12) becomes

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - w_0 - \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}_n)\}^2.$$
 (3.18)

Setting the derivative with respect to  $w_0$  equal to zero, and solving for  $w_0$ , we obtain

$$w_0 = \overline{t} - \sum_{j=1}^{M-1} w_j \overline{\phi_j} \tag{3.19}$$

where we have defined

$$\overline{t} = \frac{1}{N} \sum_{n=1}^{N} t_n, \qquad \overline{\phi_j} = \frac{1}{N} \sum_{n=1}^{N} \phi_j(\mathbf{x}_n). \qquad (3.20)$$

Thus the bias  $w_0$  compensates for the difference between the averages (over the training set) of the target values and the weighted sum of the averages of the basis function values.

## MULTIPLE OUTPUTS

- What if we have a vector of *d*-outputs rather than a single one, i.e. what if observations X, T are (x<sub>i</sub>, t<sub>i</sub>)<sub>*l*=1,...,N</sub>?
- If we use separate weights for each output dimension,  $\mathbf{W} = (w_{ij})$ , then the model is

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

which is easily seen to factorise in the different outputs, so that we need to solve *d* independent ML problems, giving

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

• Generalise to the case in which some coefficients of **W** are shared among outputs (i.e., constrained to be equal).

## AN EXAMPLE (BISHOP)

• As an example, consider data generated by the model  $t = sin(2\pi x) + \epsilon$ , from which we generate few observations:



• We want to fit a polynomial model of degree *M*, where *M* is to be chosen:

$$y(x,\mathbf{w}) = w_0 x^0 + w_1 x^1 + \ldots + w_M x^M$$

## AN EXAMPLE (BISHOP)

Max likelihood solution for different M



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## AN EXAMPLE (BISHOP)

- For *M* = 9 we face the problem of overfitting: the model is too complex ML explains noise rather than data.
- To validate a model, we need test data, different from the train data. Then we can compute the root mean square error on test (and train) data.

$$E_{RMS} = \sqrt{2E_D(\mathbf{w_{ML}})/N}$$



# AN EXAMPLE (BISHOP)

 Overfitting depends also on how many observations: the more observations, the less overfitting:



The fine-tuning of model to data reflects usually in large coefficients.

	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
$w_7^{\star}$				1042400.18
$w_8^{\star}$				-557682.99
$w_9^{\star}$				125201.43

## **REGULARISED MAXIMUM LIKELIHOOD**

- One way to avoid overfitting is to penalise solutions with large values of coefficients **w**.
- This can be enforced by introducing a regularisation term on the error function to be minimised:

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

- λ > 0 is the regularisation coefficient, and governs how strong is the penalty.
- A common choice is

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

known as ridge regression, with solution

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

## **REGULARISED MAXIMUM LIKELIHOOD**

• A more general form of the penalty term is

$${\sf E}_W({f w})=rac{1}{2}\sum_j |w_j|^q$$

- q = 2 is the ridge regression, while q = 1 is the lasso regression.
- Lasso regression has the property that it produces sparse models as some coefficients tend to be set to zero. However, it has no analytic solution.



## EXAMPLE: REGULARISED ML

• Let's consider the sine example, and fit the model of degree M = 9 by ridge regression, for different  $\lambda' s$ .



 If we compute the RMSE on a test set, we can see how the error changes with λ



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# TRAIN, VALIDATION, AND TEST DATA

- The regularisation coefficient *λ* is a method parameter. But how can we set it?
- Ideally, we should divide our data in a train set, a test set, and a validation set, which can be used to set method's parameters.
- Often, we do not have all such data, hence we can resort to cross-validation

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- Often, we do not have all such data, hence we can resort to cross-validation
- *n*-fold cross-validation: split data set in *n* blocks, use in turn each block for validation and the rest for training, average the error on the *n* runs.
- leave one out cross-validation: validate in tuns on a single data point left out from the training set and average.

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#### EXPECTED LOSS

 If we have a model p(x, t) of input-output, one way to make a prediction (choose t\* given x\*) is by minimising an expected loss functional

$$\mathbb{E}[L] = \iint \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) \,\mathrm{d}\mathbf{x} \,\mathrm{d}t.$$
(1.87)

• The solution for the square loss functional is the conditional expectation

$$y(\mathbf{x}) = \frac{\int tp(\mathbf{x}, t) \,\mathrm{d}t}{p(\mathbf{x})} = \int tp(t|\mathbf{x}) \,\mathrm{d}t = \mathbb{E}_t[t|\mathbf{x}]$$
(1.89)

• This can be seen by summing and subtracting  $\mathbb{E}[t|\mathbf{x}]$  inside the integral, getting

$$\mathbb{E}[L] = \int \left\{ y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}] \right\}^2 p(\mathbf{x}) \, \mathrm{d}\mathbf{x} + \int \left\{ \mathbb{E}[t|\mathbf{x}] - t \right\}^2 p(\mathbf{x}) \, \mathrm{d}\mathbf{x}.$$
(1.90)

#### **BIAS VARIANCE DECOMPOSITION**

- If we do not have the full model, but only observe a dataset D, then we can try to find the best approximant to the true conditional expectation, y(x, D).
- To test a method, we can try to generate many datasets and take the average E<sub>D</sub> w.r.t. the dataset. After some computations, calling h(x) the true conditional expectation:

expected loss = 
$$(bias)^2 + variance + noise$$
 (3.41)

where

$$(\text{bias})^2 = \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 p(\mathbf{x}) \,\mathrm{d}\mathbf{x}$$
 (3.42)

variance = 
$$\int \mathbb{E}_{\mathcal{D}} \left[ \{ y(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})] \}^2 \right] p(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$
 (3.43)

noise = 
$$\int {\{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t}$$
 (3.44)

#### **EXAMPLE: BIAS VARIANCE DECOMPOSITION**

left: solutions for individual datasets

right: averages over datasets



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## EXAMPLE: BIAS VARIANCE DECOMPOSITION

• For the sine example, we can compute bias and variance as a function of the regularisation coefficient. The trade off is evident.











#### THE BAYESIAN APPROACH

- Regularisation works by biasing
- One way to bias estimators is to have prior beliefs and being Bayesian
- Let's assume the regression weights have a Gaussian prior
   w ~ N(0, αl) and that the bias is zero
- The posterior is given by Bayes theorem:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \alpha, \beta) = \frac{p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \alpha, \beta)p(\mathbf{w}|\alpha)}{p(\mathbf{t}|\mathbf{X}, \alpha, \beta)}$$

#### THE POSTERIOR DISTRIBUTION

• Hence, the log posterior is

$$\log p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \alpha, \beta) = -\frac{\beta}{2} \sum_{j=1}^{N} [t_j - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_j)]^2 - \alpha \mathbf{w}^T \mathbf{w} + const$$

• As it is a quadratic function in w, it is the log of a Gaussian:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(\mathbf{w}|\mathbf{m}_{\mathbf{N}}, \mathbf{S}_{\mathbf{N}})$$

with mean and variance

$$\mathbf{m}_{\mathbf{N}} = \beta \mathbf{S}_{\mathbf{N}} \mathbf{\Phi}^{\mathsf{T}} \mathbf{t}$$

$$\mathbf{S_N}^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi}$$

Alternatively: use the formula for the product of two gaussians.

#### THE POSTERIOR DISTRIBUTION

In general, we can take a general Gaussian prior

 $\rho(\textbf{w}|\textbf{m_0},\textbf{S_0}) = \mathcal{N}(\textbf{w}|\textbf{m_0},\textbf{S_0})$ 

This will result in a Gaussian posterior
 p(w|X, t, α, β) = N(w|m<sub>N</sub>, S<sub>N</sub>) with

$$\mathbf{m}_{\mathbf{N}} = \mathbf{S}_{\mathbf{N}} [\mathbf{S}_{\mathbf{0}}^{-1} \mathbf{m}_{\mathbf{0}} + \beta \mathbf{\Phi}^{T} \mathbf{t}]$$
$$\mathbf{S}_{\mathbf{N}}^{-1} = \mathbf{S}_{\mathbf{0}}^{-1} + \beta \mathbf{\Phi}^{T} \mathbf{\Phi}$$

# **POSTERIOR UPDATE**



#### THE PREDICTIVE DISTRIBUTION

 Given the posterior, one can find the MAP estimate. However, in a fully Bayesian treatment, one makes predictions by integrating out the parameters via their posterior distribution.

$$p(t|\mathbf{t}, \alpha, \beta) = \int p(t|\mathbf{t}, \mathbf{w}, \alpha, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) d\mathbf{w}$$

The predictive distribution is still a Gaussian

$$p(t|\mathbf{t},\alpha,\beta) = \mathcal{N}(t|\mathbf{m}_{\mathsf{N}}^{\mathsf{T}}\boldsymbol{\phi}(\mathbf{x}),\sigma_{\mathcal{N}}^{2}(\mathbf{x}))$$

with mean  $\mathbf{m}_{\mathbf{N}}^{T} \boldsymbol{\phi}(\mathbf{x})$  and variance

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^T \mathbf{S}_{\mathbf{N}} \boldsymbol{\phi}(\mathbf{x})$$

• It can be shown that  $\sigma_{N+1}^2(\mathbf{x}) \le \sigma_N^2(\mathbf{x})$  and  $\sigma_N^2(\mathbf{x}) \to 1/\beta$
## EXAMPLE



## EXAMPLE



## MARGINAL LIKELIHOOD

- The marginal likelihood *p*(t|*α*, *β*), appearing at the denominator in Bayes theorem, can be used to identify good *α* and *β*, known as hyperparameters.
- Intuitively, we can place a prior distribution over α and β, compute their posterior, and use this in a fully Bayesian treatment of the regression:

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

 If we assume the posterior is peaked around the mode, then we can take the MAP as an approximation of the full posterior for α and β. If the prior is flat, this will boil down to the ML solution.

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# MARGINAL LIKELIHOOD

 Hence we need to optimise the marginal likelihood, which can be computed as:

$$\log p(\mathbf{t}|\alpha,\beta) = \frac{M}{2} \log \alpha + \frac{N}{2} \log \beta - E(\mathbf{m}_{\mathbf{N}}) - \frac{1}{2} \log |\mathbf{S}_{\mathbf{N}}^{-1}| - \frac{N}{2} \log 2\pi$$

with

$$\mathcal{E}(\mathbf{m}_{\mathbf{N}}) = rac{eta}{2} \|\mathbf{t} - \mathbf{\Phi}\mathbf{m}_{\mathbf{N}}\|^2 + rac{lpha}{2} \mathbf{m}_{\mathbf{N}}^{T} \mathbf{m}_{\mathbf{N}}$$

 This optimisation problem can be solved with any optimisation routine, or with specialised methods.

## **OPTIMISING THE MARGINAL LIKELIHOOD**

- We will present a fix-point algorithm: we will write the gradient equations equal to zero as fix-point equations and iterate until convergence.
- In taking the derivative w.r.t α or β, the most challenging term is the log of the determinant of S<sub>N</sub><sup>-1</sup> = αI + βΦ<sup>T</sup>Φ.
- To deal with it, let  $\lambda_i$  be the eigenvalues of  $\beta \Phi^T \Phi$ , so that  $|\mathbf{S}_{\mathbf{N}}^{-1}| = \prod_{i=0}^{M-1} (\alpha + \lambda_i).$
- We then have that

$$\partial \log |\mathbf{S_N}^{-1}| / \partial \alpha = \sum_i \frac{1}{\alpha + \lambda_i}$$

• Moreover,  $\lambda_i$  are proportional to  $\beta$ , so that  $\partial \lambda_i / \partial \beta = \lambda_i / \beta$ 

#### **OPTIMISING THE MARGINAL LIKELIHOOD**

• Now, define

$$\gamma = \sum_{i} \frac{\lambda_i}{\alpha + \lambda_i}$$

(which measures the number of well determined parameters)

 By deriving the log-marginal w.r.t. α and setting derivative to zero, we obtain:

$$\alpha = \frac{\gamma}{\mathbf{m}_{\mathsf{N}}{}^{\mathsf{T}}\mathbf{m}_{\mathsf{N}}} = g_{\alpha}(\alpha,\beta)$$

 By deriving the log-marginal w.r.t. β and setting derivative to zero, we obtain:

$$\frac{1}{\beta} = \frac{1}{N - \gamma} \sum_{n=1}^{\infty} N[t_n - \mathbf{m_N}^T \boldsymbol{\phi}(\mathbf{x_n})]^2 = \frac{1}{g_{\beta}(\alpha, \beta)}$$

• We start from an initial value  $\alpha_0$  and  $\beta_0$  and iterate  $\alpha_{n+1} = g_{\alpha}(\alpha_n, \beta_n), \beta_{n+1} = g_{\beta}(\alpha_n, \beta_n)$  until convergence.

## BAYESIAN MODEL COMPARISON

- Consider M<sub>1</sub> and M<sub>2</sub> two different models, which one is the best to explain the data D?
- In a Bayesian setting, we may place a prior p(M<sub>j</sub>) on the models, and compute the posterior p(M<sub>j</sub>|D) = p(D|M<sub>j</sub>)p(M<sub>j</sub>)/Σ<sub>j</sub> p(D|M<sub>j</sub>)p(M<sub>j</sub>).
- As we typically have additional parameters  $\mathbf{w}$ , the term  $p(\mathcal{D}|\mathcal{M}_j)$  is the model evidence/ marginal likelihood.
- The ratio  $p(\mathcal{D}|\mathcal{M}_1)/p(\mathcal{D}|\mathcal{M}_2)$  is known as Bayes Factor.

#### BAYESIAN MODEL COMPARISON

- In Bayesian model comparison, we can take two approaches.
- We can compute the predictive distribution for each model and average it by the posterior model probability

$$p(\mathbf{t}|\mathcal{D}) = \sum_{j} p(\mathbf{t}|\mathcal{M}_{j}, \mathcal{D}) p(\mathcal{M}_{j}|\mathcal{D})$$

• Alternatively, we can choose the model with larger Bayes Factor. This will pick the correct model on average. In fact, the average log Bayes factor (assuming  $\mathcal{M}_1$  is the true model) is

$$\int p(\mathcal{D}|\mathcal{M}_1) \log \frac{p(\mathcal{D}|\mathcal{M}_1)}{p(\mathcal{D}|\mathcal{M}_2)} > 0$$

## OUTLINE







## DUAL REPRESENTATION

- Consider a regression problem with data (**x**<sub>i</sub>, *y<sub>i</sub>*), and a linear model **w**<sup>T</sup>φ(**x**).
- We can restrict the choice of w to the linear subspace spanned by φ(x<sub>1</sub>),...,φ(x<sub>N</sub>), as any w<sub>⊥</sub> othogonal to this subspace will give a contribution w<sub>⊥</sub><sup>T</sup>φ(x<sub>i</sub>) = 0 on input points:

$$\mathbf{w} = \sum_{j=1}^N a_j \boldsymbol{\phi}(\mathbf{x_j})$$

- a are known as the dual variables
- By defining the kernel  $k(\mathbf{x}_i, \mathbf{x}_j) := \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ , we can write

$$\mathbf{w}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}_{i}) = \mathbf{a}^{\mathsf{T}} \mathbf{K}^{i}$$

Where  $\mathbf{K}^{\mathbf{i}}$  is the *i*th column of the Gram matrix  $\mathbf{K}$ ,  $K_{ij} = k(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}})$ .

#### DUAL REGRESSION PROBLEM

 In the dual variables, we have to optimise the following regression equation

$$E_d(\mathbf{a}) + \lambda E_W(\mathbf{a}) = \sum_{i=1}^N (t_i - \mathbf{a}^T \mathbf{K}^i)^2 + \lambda \mathbf{a}^T \mathbf{K} \mathbf{a}^T$$

 By deriving w.r.t a and setting the gradient to zero, we obtain the solution

$$\hat{\mathbf{a}} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}$$

• At a new input **x**\*, the prediction will then be

$$y(\mathbf{x}^*) = \mathbf{k}_*^{T} (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}$$
  
with  $\mathbf{k}_*^{T} = (k(\mathbf{x}^*, \mathbf{x}_1), \dots, k(\mathbf{x}^*, \mathbf{x}_N))$ 

## THE KERNEL TRICK

- The dual objective function depends only on the scalar product of input vectors
- We can replace the Euclidean scalar product with *any* (non-linear) scalar product
- This is usually obtained by giving directly a non-linear kernel function k(x<sub>i</sub>, x<sub>j</sub>) (kernel trick)
- This enables us to work with more general set of basis functions, even countable. See Gaussian processes.
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- This enables us to work with more general set of basis functions, even countable. See Gaussian processes.
- The same dual procedure applies to other algorithms, notably linear classification and SVMs
- The computational cost to solve the primal problem is  $O(M^3)$ , while the dual costs  $O(N^3)$ . They can be both prohibitive is *N* and *M* are large. In this case, one can optimise the log likelihood directly, using gradient based methods.