Linear regression

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Motivation

Estimate the outcome of the random vector $\mathbf{x}$ based on the noisy observations on the outcome of the random variable $t = f(\mathbf{x}) + \epsilon$.

Linear Regression

1. Linear Regression-Parametric approach
2. Maximum Likelihood approach
3. Least square estimation
4. Regularization technique
5. Error in Regression= $Bias^2 + var + Noise$
6. Bayes technique
7. Kernel smoothing

Linear regression-Parametric approach

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2. $\mathbf{t}$ is the observation and ϵ is Guassian distributed random variable with mean zero and variance $\frac{1}{\beta}$

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4. Let us assume that the basis functions $\phi_0(\mathbf{x}), \phi_1(\mathbf{x}), \phi_2(\mathbf{x}) \cdots \phi_{M-1}(\mathbf{x})$ are known.
5. The requirement is to estimate obtain the optimal value of $\mathbf{w}$

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5. $\mathbf{w}$ is estimated as the conditional mean of the posterior density function $f(\mathbf{w}/\mathbf{t}, \mathbf{x})$

Maximum Likelihood Estimation

1. MAP Estimate: $\mathbf{w}$ is estimated that maximizes the posterior density function $f(\mathbf{w}/\mathbf{t}, \mathbf{x})$
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5. The optimal value of $\mathbf{w}$ is estimated that maximizes the likelihood function $f(\mathbf{t}/\mathbf{w}, \mathbf{x})$

Maximum Likelihood Estimation

1. Thus optimal value of $\mathbf{w}$ is estimated that maximizes the likelihood function $f(\mathbf{t}/\mathbf{w}, \mathbf{x})$
2. THIS IS KNOWN AS MAXIMUM LIKELIHOOD ESTIMATION

Likelihood function with N observations

$$f(t_1 t_2 \cdots t_N / \mathbf{w}, \mathbf{x}) = K \prod_{i=1}^{i=N} e^{-\frac{(t_i - w^T \phi(x_i))^2}{2\sigma^2}} \tag{1}$$

1. As logarithm is the increasing function, Maximizing Likelihood function is equivalent to maximizing the logarithm of the Likelihood function
2. Taking logarithm of (1), we get the following.

$$\ln(f(t_1 t_2 \cdots t_N / \mathbf{w}, \mathbf{x})) = -\sum_{i=1}^{i=N} \frac{(t_i - w^T \phi(x_i))^2}{2\sigma^2} + lnK \tag{2}$$

Maximum Likelihood versus Least square solution

$$\ln(f(t_1 t_2 \cdots t_N / \mathbf{w}, \mathbf{x})) = -\sum_{i=1}^{i=N} \frac{(t_i - w^T \phi(x_i))^2}{2\sigma^2} + lnK \tag{3}$$

1. Maximizing (2) is equivalent to minimizing the following.

$$\frac{(t_i - w^T \phi(x_i))^2}{2\sigma^2} \tag{4}$$

2. This is the Least square solution

Matrix Representation

This can be written in the matrix form as follows.

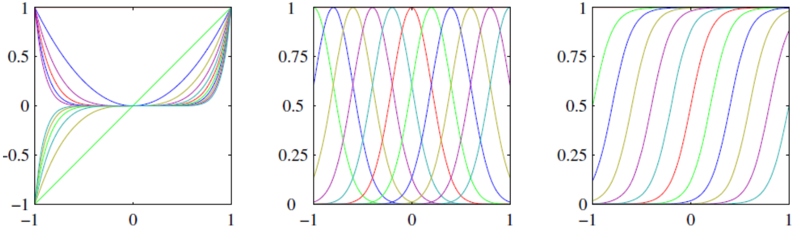
$$\begin{bmatrix} \phi_0(x_1) & \cdots & \phi_{M-1}(x_1) \\ \phi_0(x_2) & \cdots & \phi_{M-1}(x_2) \\ \cdots & \cdots & \cdots \\ \phi_0(x_N) & \cdots & \phi_{M-1}(x_N) \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{M-1} \end{bmatrix} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ \vdots \\ t_N \end{bmatrix} \tag{5}$$

This is represented as follows. $\mathbf{\Phi w} = \mathbf{t}$The solution is obtained using pseudo inverse as $\hat{w} = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{t}$

Observation

1. We understand that Maximum Likelihood estimation is identical as that of the Least square estimation (?) $\cdots$

Basis function



Examples of basis functions, showing polynomials on the left, Gaussians of the form in the centre, and sigmoidal of the form on the right.

$$\phi_j(x) = x^j \qquad \phi_j(x) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\} \qquad \phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$$

$$\sigma(a) = \frac{1}{1+\exp(-a)} \qquad \tanh(a) = 2\sigma(a) - 1$$

Prediction distribution

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

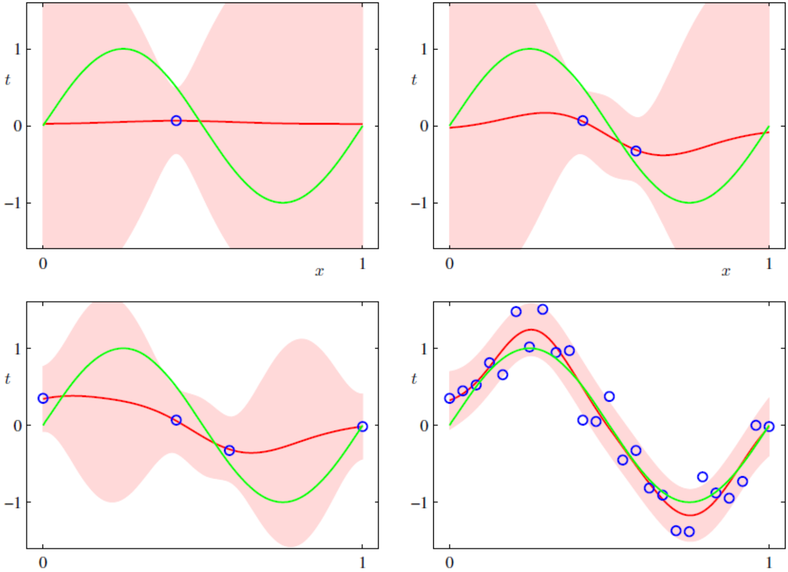
$$p(t|\mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

where the variance $\sigma_N^2(\mathbf{x})$ of the predictive distribution is given by

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

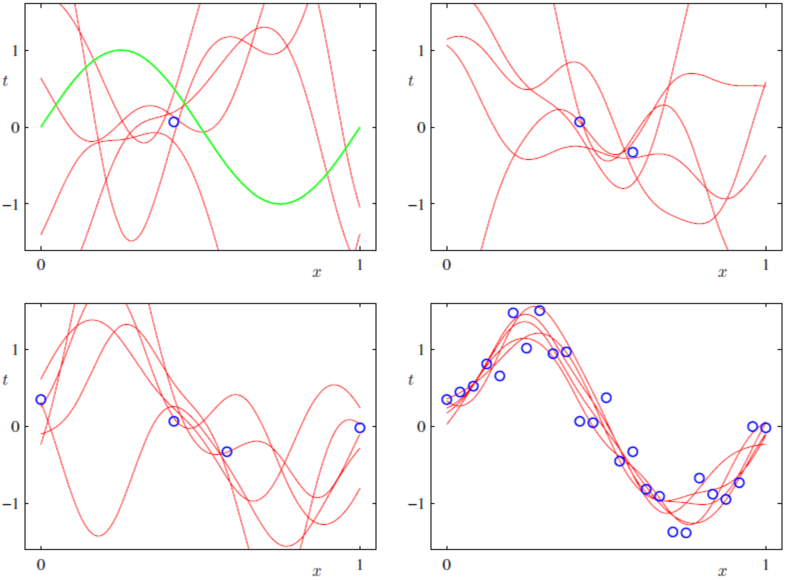
$$\sigma_{N+1}^2(\mathbf{x}) \leqslant \sigma_N^2(\mathbf{x}).$$

Prediction distribution



Examples of the predictive distribution (3.58) for a model consisting of 9 Gaussian basis functions

Prediction distribution



Plots of the function $y(x, \mathbf{w})$ using samples from the posterior distributions over $\mathbf{w}$ corresponding to the plots in Figure

Regularization techniques.

1. The observation $t = \mathbf{w}^T \phi(\mathbf{x}) + \epsilon$ is the parametric model.
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2. $f(\mathbf{w})$ is the prior density function
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5. They are related using Bayes as follows.

$$f(\mathbf{t}/\mathbf{w}) = \frac{f(\mathbf{t}/\mathbf{w})f(\mathbf{w})}{f(\mathbf{t})} \tag{6}$$

Regularization techniques

1. It is observed that $f(\mathbf{t}/\mathbf{w})$ is modelled as Gaussian distributed with mean $\mathbf{w}^T\phi(x)$ and variance $\frac{1}{\beta}$
2. In Likelihood estimation, $f(\mathbf{w})$ is uniform distributed and hence maximizing $f(\mathbf{w}/\mathbf{t})$ (MAP) is identical as that of maximizing $f(\mathbf{t}/\mathbf{w})$
3. This is known as Maximum Likelihood estimation
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5. This ends up solving the matrix $\Phi\mathbf{w} = \mathbf{t}$

Regularization Techniques

1. $$\begin{bmatrix} \phi_0(x_1) & \cdots & \phi_{M-1}(x_1) \\ \phi_0(x_2) & \cdots & \phi_{M-1}(x_2) \\ \cdots & \cdots & \cdots \\ \phi_0(x_N) & \cdots & \phi_{M-1}(x_N) \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{M-1} \end{bmatrix} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ \vdots \\ t_N \end{bmatrix} \tag{7}$$
2. Using pseudo inverse computation **w** is estimated as the following.
$$\mathbf{w} = (\Phi^T\Phi)^{-1}\Phi^T\mathbf{t} \tag{8}$$
3. From the above, it is understood that the estimated vector **w** is data dependent
4. Ends up with Overfitting.

Regularization

1. To circumvent this, the Least square problem is formulated with the constraints $\sum_{n=1}^{n=M} |w_n|^2 \leq \eta$ as given below.

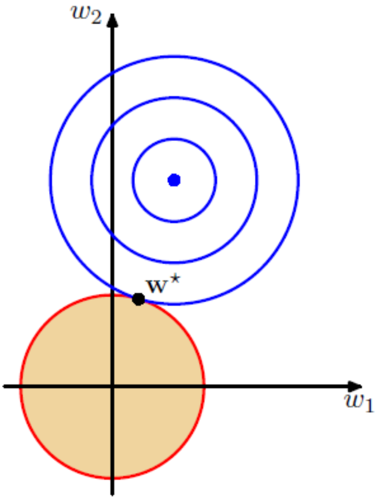
$$J = \frac{1}{2}\sum_{n=1}^{n=N}(t_n - \mathbf{w}^T\phi(\mathbf{x}))^2 + \frac{\lambda}{2}\sum_{n=1}^{n=M}|w_n|^2$$

2. The estimate is given as the following.

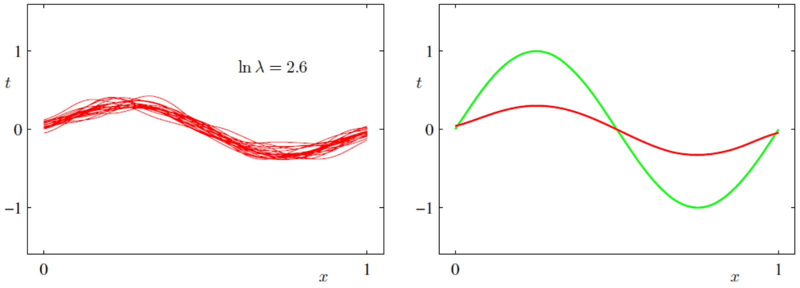
$$\mathbf{w} = (\Phi^T\Phi + \lambda I)^{-1}\Phi^T\mathbf{t} \tag{9}$$

3. λ is known as Regularization constant.

Regularization

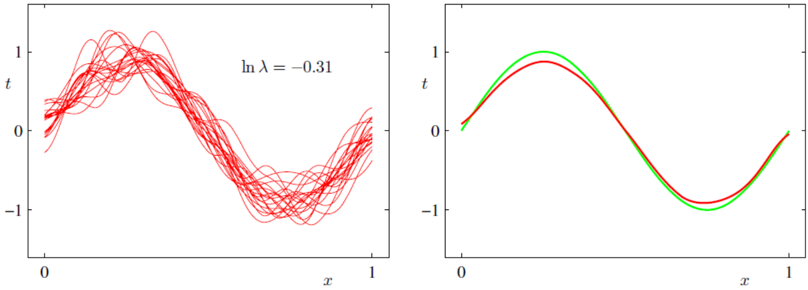


Regularization



1. Number of datasets (L) =100
2. Number of data points (N) =25
3. Number of Gaussian basis functions=24, i.e $M = 25$

Regularization



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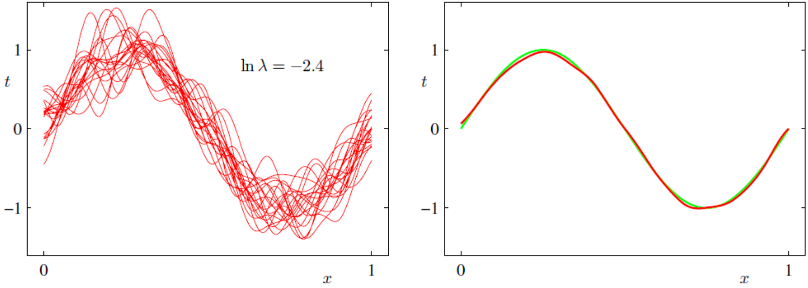

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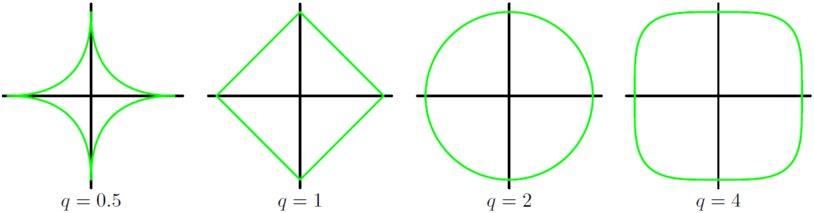


Contours of the regularization term in for various values of the parameter q.

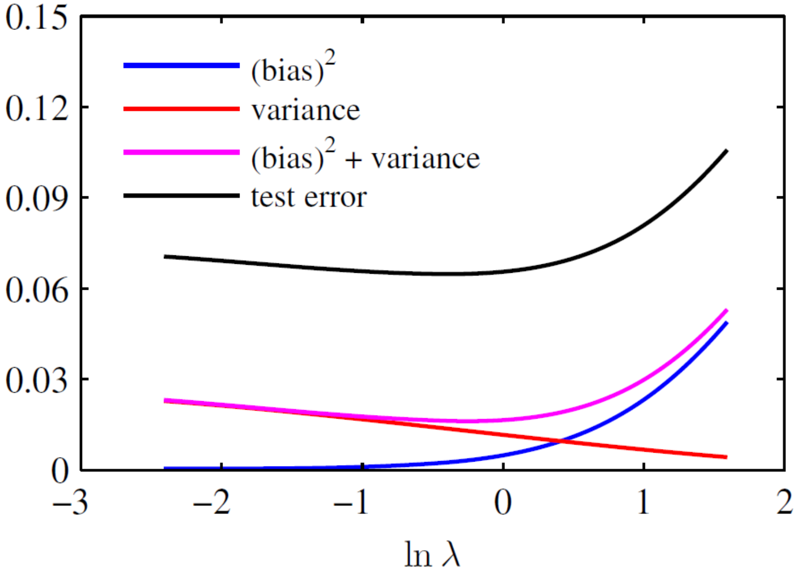
$\text{Bias}^2 + \text{Variance}$

$$\overline{y}(x) = \frac{1}{L}\sum_{l=1}^{L} y^{(l)}(x)$$

$$(\text{bias})^2 = \frac{1}{N}\sum_{n=1}^{N}\{\overline{y}(x_n) - h(x_n)\}^2$$

$$\text{variance} = \frac{1}{N}\sum_{n=1}^{N}\frac{1}{L}\sum_{l=1}^{L}\left\{y^{(l)}(x_n) - \overline{y}(x_n)\right\}^2$$

$Bias^2 + Variance$



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Bayes technique to estimate $\mathbf{w}$ in parametric approach based Linear regression.

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1. Using pseudo inverse computation **w** is estimated as the following.
$$\mathbf{w} = (\Phi^T\Phi)^{-1}\Phi^T\mathbf{x} \tag{11}$$
2. What if **w** is assumed as Multivariate Gaussian density function?

Bayes technique to estimate $\mathbf{w}$ in parametric approach based Linear regression

1. If the prior density function $f(\mathbf{w})$ is assumed as Multivariate Gaussian density function with mean $\mathbf{m_o}$ and co-variance matrix $\mathbf{S_o}$.
2. Then the Aposterior density function of $\mathbf{w}$ given $\mathbf{t}$ is also Gaussian with mean vector $\mathbf{m_N}$ and co-variance matrix $\mathbf{S_N}$ as shown below.

$$\mathbf{m_N} = \mathbf{S_N}(\mathbf{S_o}^{-1} m_o + \beta \mathbf{\Phi}^\mathbf{T} \mathbf{t})$$
$$\mathbf{S_N} = (\mathbf{S_o}^{-1} + \beta(\mathbf{\Phi}^\mathbf{T}\mathbf{\Phi}))^{-1}$$

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3. What is the Conditional mean , Conditional median and the Conditional mode estimate of the posterior density function $f(\mathbf{w}/\mathbf{t})$?

Bayes technique to estimate **w** in parametric approach based Linear regression

1. Consider the case when $\mathbf{m_o}$ is zero vector and the covariance matrix is diagonal as shown below.

$$S_o = \frac{1}{\alpha} I \tag{12}$$

2.

$$\mathbf{m_N} = \beta \mathbf{S_N} \mathbf{\Phi^T t}$$
$$\mathbf{m_N} = \beta((\mathbf{S_o}^{-1} + \beta(\mathbf{\Phi^T \Phi}))^{-1})^{-1} \mathbf{\Phi^T t}$$
$$\mathbf{m_N} = \beta(\alpha \mathbf{I} + \beta(\mathbf{\Phi^T \Phi}))^{-1} \mathbf{\Phi^T t}$$

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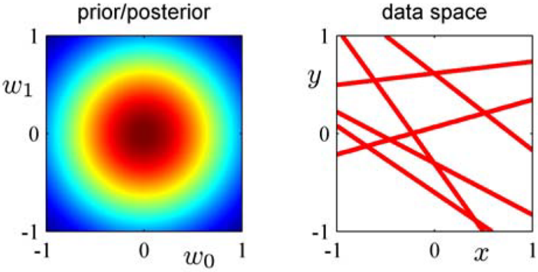
$$\mathbf{m_N} = \beta(\alpha \mathbf{I} + \beta(\mathbf{\Phi}^\mathbf{T}\mathbf{\Phi}))^{-1}\mathbf{\Phi}^\mathbf{T} \mathbf{t}$$
$$\mathbf{m_N} = (\mathbf{\Phi}^\mathbf{T}\mathbf{\Phi} + \frac{\alpha}{\beta}\mathbf{I})^{-1}\mathbf{\Phi}^\mathbf{T} \mathbf{t}$$

Bayes technique to estimate **w** in parametric approach based Linear regression

1. $\mathbf{w} = \mathbf{m_N} = (\mathbf{\Phi^T \Phi} + \frac{\alpha}{\beta}\mathbf{I})^{-1}\mathbf{\Phi^T t}$
2. This solution can be viewed as the Regularized least square solution with $\lambda = \frac{\alpha}{\beta}$

Bayes technique to estimate **w** in parametric approach based Linear regression

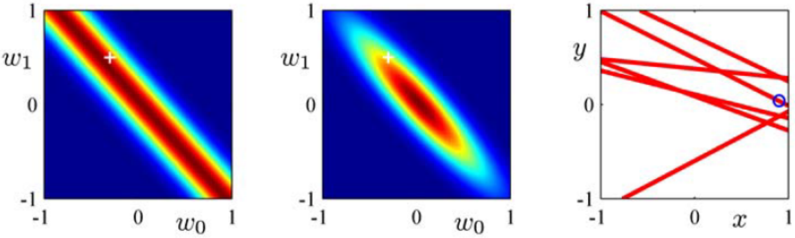


$$y(x, \mathbf{w}) = w_0 + w_1 x$$

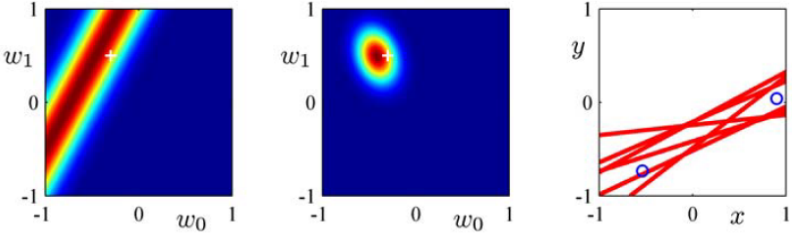
$$\beta = (1/0.2)^2 = 25$$

$$\alpha = 2.0$$

Bayes technique to estimate **w** in parametric approach based Linear regression



Bayes technique to estimate **w** in parametric approach based Linear regression



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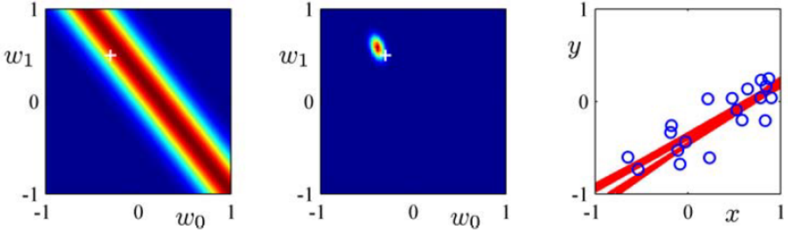


Kernel smoothing

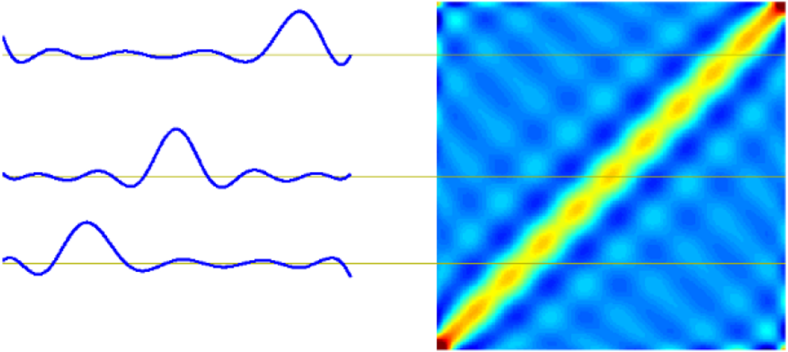
$$y(\mathbf{x}, \mathbf{m}_N) = \mathbf{m}_N^{\mathrm{T}} \phi(\mathbf{x}) = \beta \phi(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \mathbf{\Phi}^{\mathrm{T}} \mathbf{t} = \sum_{n=1}^{N} \beta \phi(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \phi(\mathbf{x}_n) t_n$$

$$y(\mathbf{x}, \mathbf{m}_N) = \sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) t_n$$

$$k(\mathbf{x}, \mathbf{x}') = \beta \phi(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \phi(\mathbf{x}')$$

is known as the *smoother matrix* or the *equivalent kernel*.

Kernel smoothing



Reference

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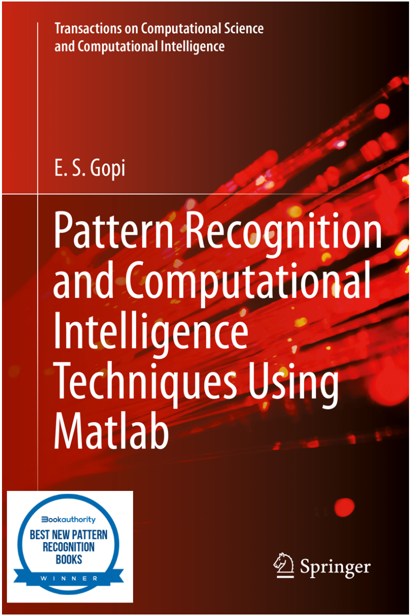
Book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