Introduction to Statistical Machine Learning

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

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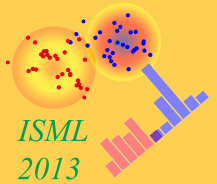

Outlines

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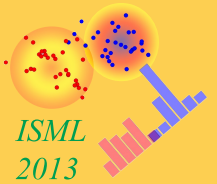
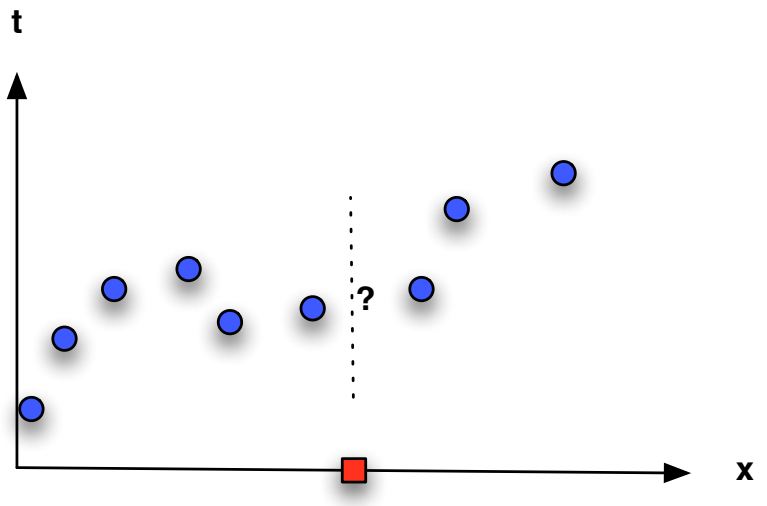


Part V

Linear Regression 1

Regression

- Given a training data set of N observations $\{\mathbf{x}_n\}$ and target values t_n.
- Goal : Learn to predict the value of one ore more target values t given a new value of the input $\mathbf{x}$.
- Example: Polynomial curve fitting (see Introduction).



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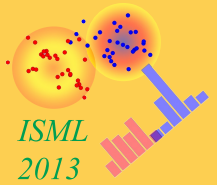
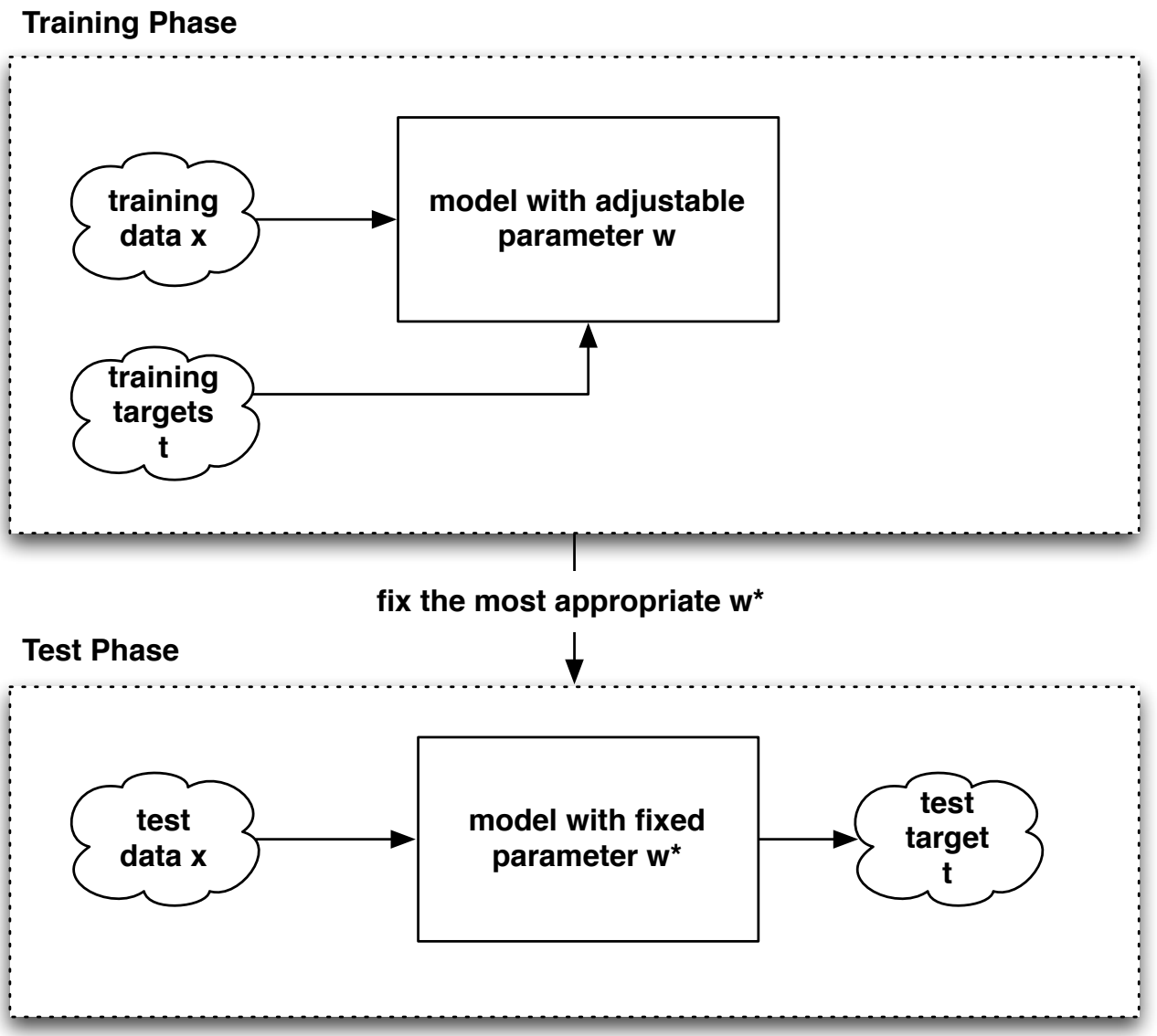


Supervised Learning



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Linear Basis Function Models

- Linear combination of fixed nonlinear basis functions

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

- parameter $\mathbf{w} = (w_0, \ldots, w_{M-1})^T$
- basis functions $\boldsymbol{\phi}(\mathbf{x}) = (\phi_0(\mathbf{x}), \ldots, \phi_{M-1}(\mathbf{x}))^T$
- convention $\phi_0(\mathbf{x}) = 1$
- w_0 is the bias parameter

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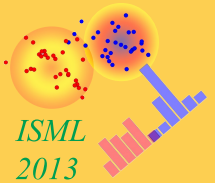
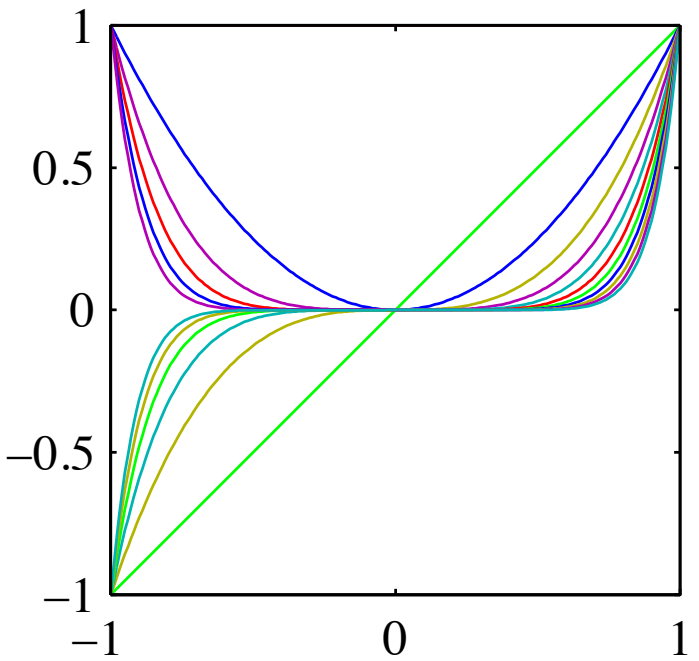


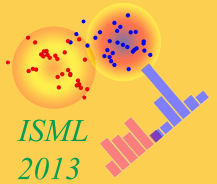
Polynomial Basis Functions

- Scalar input variable x

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

- Limitation : Polynomials are global functions of the input variable x.
- Extension: Split the input space into regions and fit a different polynomial to each region (spline functions).



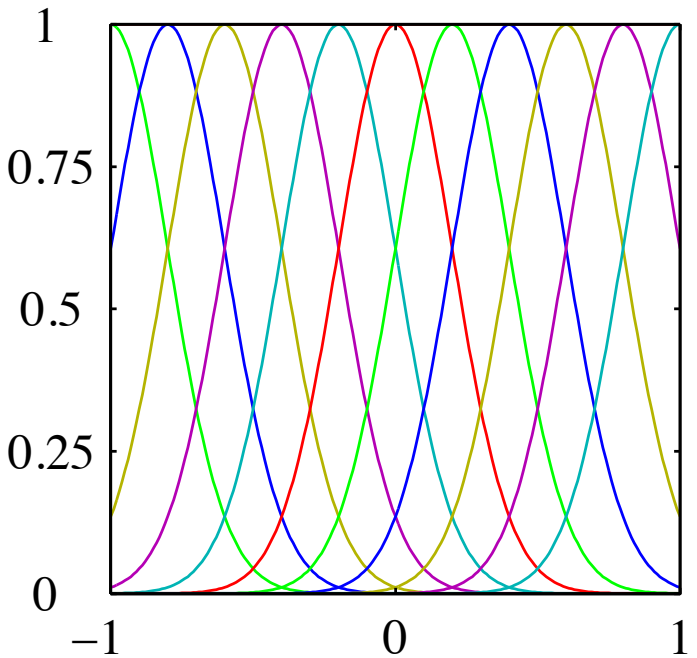


'Gaussian' Basis Functions

- Scalar input variable x

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

- Not a probability distribution.
- No normalisation required, taken care of by the model parameters w.



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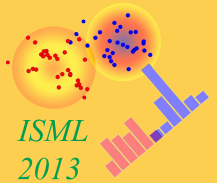


Sigmoidal Basis Functions

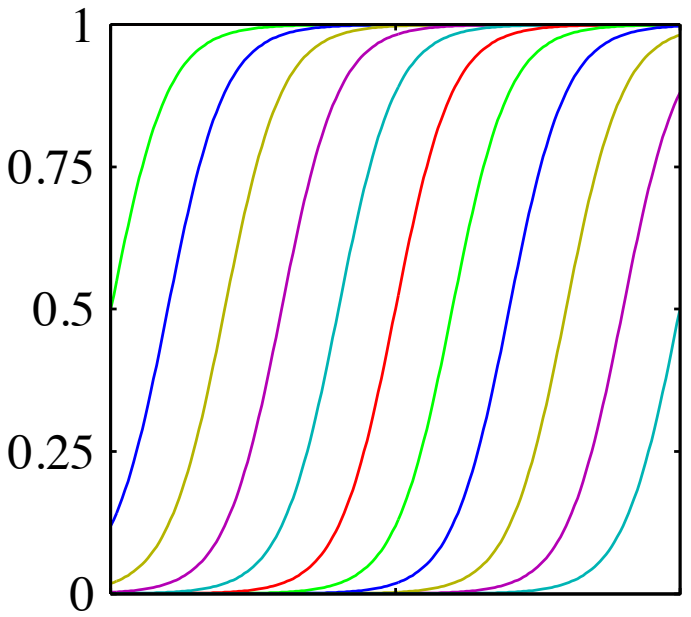
- Scalar input variable x

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

where $\sigma(a)$ is the logistic sigmoid function defined by

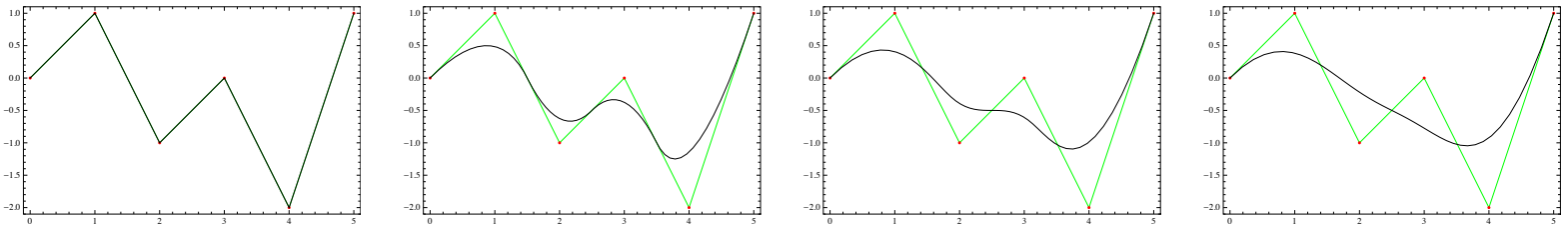
$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

- $\sigma(a)$ is related to the hyperbolic tangent $\tanh(a)$ by $\tanh(a) = 2\sigma(a) - 1$.



Other Basis Functions

- Fourier Basis : each basis function represents a specific frequency and has infinite spatial extent.
- Wavelets : localised in both space and frequency (also mutually orthogonal to simplify appliciation).
- Splines (piecewise polynomials restricted to regions of the input space; additional constraints where pieces meet, e.g. smoothness constraints $\rightarrow$ conditions on the derivatives).



Linear Splines | Quadratic Splines | Cubic Splines | Quartic Splines

Approximate the points $\{(0,0),(1,1),(2,-1),(3,0),(4,-2),(5,1)\}$ by different splines.

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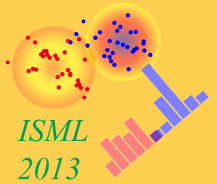

Maximum Likelihood and Least Squares

- No special assumption about the basis functions $\phi_j(\mathbf{x})$. In the simplest case, one can think of $\phi_j(\mathbf{x}) = \mathbf{x}$.
- Assume target t is given by

$$t = \underbrace{y(\mathbf{x}, \mathbf{w})}_{\text{deterministic}} + \underbrace{\epsilon}_{\text{noise}}$$

  where ϵ is a zero-mean Gaussian random variable with precision (inverse variance) β.
- Thus

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

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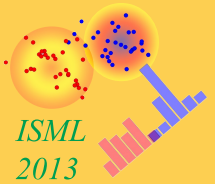

Maximum Likelihood and Least Squares

- Likelihood of one target t given the data $\mathbf{x}$

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

- Set of inputs $\mathbf{X}$ with corresponding target values $\mathbf{t}$.
- Assume data are independent and identically distributed (i.i.d.) (means : data are drawn independent and from the same distribution). The likelihood of the target $\mathbf{t}$ is then

$$\begin{aligned} p(\mathbf{t} \mid \mathbf{X}, \mathbf{w}, \beta) &= \prod_{n=1}^{N} \mathcal{N}(t_n \mid y(\mathbf{x}_n, \mathbf{w}), \beta^{-1}) \\ &= \prod_{n=1}^{N} \mathcal{N}(t_n \mid \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}) \end{aligned}$$

- From now on drop the conditioning variable $\mathbf{X}$ from the notation, as with supervised learning we do not seek to model the distribution of the input data.

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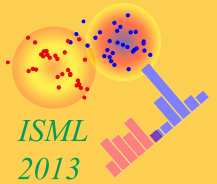

Maximum Likelihood and Least Squares

- Consider the logarithm of the likelihood $p(\mathbf{t} \mid \mathbf{w}, \beta)$ (the logarithm is a monoton function!)

$$\begin{aligned}\ln p(\mathbf{t} \mid \mathbf{w}, \beta) &= \sum_{n=1}^{N} \ln \mathcal{N}(t_n \mid \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}) \\ &= \sum_{n=1}^{N} \ln \left(\sqrt{\frac{\beta}{2\pi}} \exp \left\{ -\frac{\beta}{2} (t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n))^2 \right\} \right) \\ &= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w})\end{aligned}$$

where the sum-of-squares error function is

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

- $\arg\max_{\mathbf{w}} \ln p(\mathbf{t} \mid \mathbf{w}, \beta) \rightarrow \arg\min_{\mathbf{w}} E_D(\mathbf{w})$

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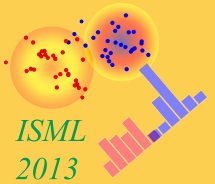

Maximum Likelihood and Least Squares

- Goal: Find a more compact representation.
- Rewrite the error function

$$E_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\boldsymbol{\phi}(x_n)\}^2 = \frac{1}{2}(\mathbf{t}-\boldsymbol{\Phi}\mathbf{w})^T(\mathbf{t}-\boldsymbol{\Phi}\mathbf{w})$$

where $\mathbf{t} = (t_1,\ldots,t_N)^T$, and

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

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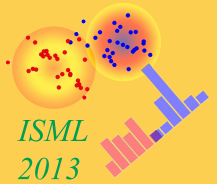

Maximum Likelihood and Least Squares

- The log likelihood is now

$$\ln p(\mathbf{t} \mid \mathbf{w}, \beta) = \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w})$$
$$= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta \frac{1}{2} (\mathbf{t} - \mathbf{\Phi w})^T (\mathbf{t} - \mathbf{\Phi w})$$

- Find critical points of $\ln p(\mathbf{t} \mid \mathbf{w}, \beta)$.
- Directional derivative in direction $\boldsymbol{\xi}$

$$\mathcal{D} \ln p(\mathbf{t} \mid \mathbf{w}, \beta)(\boldsymbol{\xi}) = \beta \boldsymbol{\xi}^T (\mathbf{\Phi}^T \mathbf{t} - \mathbf{\Phi}^T \mathbf{\Phi w})$$

shall be zero in all directions $\boldsymbol{\xi}$. Therefore

$$0 = \mathbf{\Phi}^T \mathbf{t} - \mathbf{\Phi}^T \mathbf{\Phi w},$$

- which results in

$$\mathbf{w}_{ML} = (\mathbf{\Phi}^T \mathbf{\Phi})^{-1} \mathbf{\Phi}^T \mathbf{t} = \mathbf{\Phi}^\dagger \mathbf{t}$$

where $\mathbf{\Phi}^\dagger$ is the Moore-Penrose pseudo-inverse of the matrix $\mathbf{\Phi}$.

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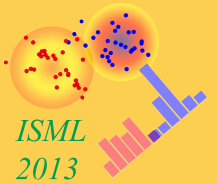

Maximum Likelihood and Least Squares

- Found a critical point $\mathbf{w}_{ML}$ for $\ln p(\mathbf{t} \mid \mathbf{w}, \beta)$. Is it a maximum, a minimum, or a saddle point?
- Calculate the second directional derivative

$$\begin{aligned}\mathcal{D}^2 \ln p(\mathbf{t} \mid \mathbf{w}, \beta)(\boldsymbol{\xi}, \boldsymbol{\xi}) &= -\beta\, \boldsymbol{\xi}^T \boldsymbol{\Phi}^T \boldsymbol{\Phi} \boldsymbol{\xi} \\ &= -\beta\, (\boldsymbol{\Phi}\boldsymbol{\xi})^T \boldsymbol{\Phi}\boldsymbol{\xi} \\ &= -\beta\, \|\boldsymbol{\Phi}\boldsymbol{\xi}\|^2 \leq 0\end{aligned}$$

- We found a maximum.
- (Is it enough to check the second directional derivative in two directions $\boldsymbol{\xi}$ which are the same? Yes, because for any bilinear function $g(\boldsymbol{\xi}, \boldsymbol{\eta})$, symmetric in its arguments,

$$\begin{aligned}&\frac{1}{2}\left[g(\boldsymbol{\xi}, \boldsymbol{\xi}) + g(\boldsymbol{\eta}, \boldsymbol{\eta}) - g(\boldsymbol{\xi} - \boldsymbol{\eta}, \boldsymbol{\xi} - \boldsymbol{\eta})\right] \\ &= \frac{1}{2}\left[g(\boldsymbol{\xi}, \boldsymbol{\xi}) + g(\boldsymbol{\eta}, \boldsymbol{\eta}) - g(\boldsymbol{\xi}, \boldsymbol{\xi}) - g(\boldsymbol{\eta}, \boldsymbol{\eta}) + g(\boldsymbol{\xi}, \boldsymbol{\eta}) + g(\boldsymbol{\eta}, \boldsymbol{\xi})\right] \\ &= \frac{1}{2}\left[g(\boldsymbol{\xi}, \boldsymbol{\eta}) + g(\boldsymbol{\eta}, \boldsymbol{\xi})\right] = g(\boldsymbol{\xi}, \boldsymbol{\eta})\end{aligned}$$

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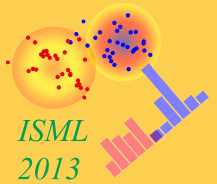

Maximum Likelihood and Least Squares

- The log likelihood with the optimal $\mathbf{w}_{ML}$ is now

$$\ln p(\mathbf{t} \mid \mathbf{w}_{ML}, \beta)$$
$$= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta \frac{1}{2} (\mathbf{t} - \mathbf{\Phi} \mathbf{w}_{ML})^T (\mathbf{t} - \mathbf{\Phi} \mathbf{w}_{ML})$$

- Find critical points of $\ln p(\mathbf{t} \mid \mathbf{w}, \beta)$ wrt β,

$$\frac{\partial \ln p(\mathbf{t} \mid \mathbf{w}_{ML}, \beta)}{\partial \beta} = 0$$

results in

$$\frac{1}{\beta_{ML}} = \frac{1}{N} (\mathbf{t} - \mathbf{\Phi} \mathbf{w}_{ML})^T (\mathbf{t} - \mathbf{\Phi} \mathbf{w}_{ML})$$

- Note: We can first find the maximum likelihood for $\mathbf{w}$ as this does not depend on β. Then we can use $\mathbf{w}_{ML}$ to find the maximum likelihood solution for β.
- Could we have chosen optimisation wrt β first, and then wrt to $\mathbf{w}$?

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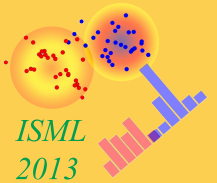
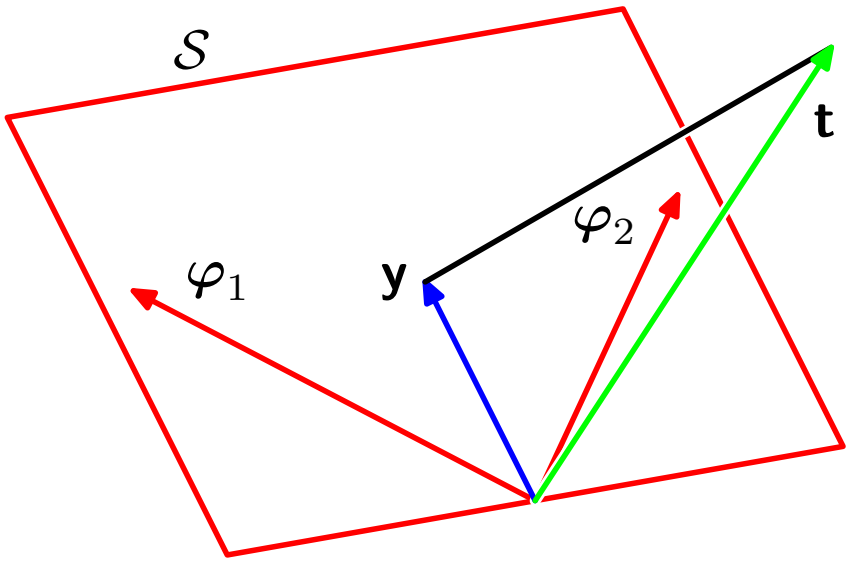


Geometry of Least Squares

- Target vector $\mathbf{t} = (t_1, \ldots, t_N)^T \in \mathbb{R}^N$
- Basis vectors $\varphi_j = (\mathbf{\Phi}_{j1}, \ldots, \mathbf{\Phi}_{jN})^T = (\phi_j(\mathbf{x}_1), \ldots, \phi_j(\mathbf{x}_N))^T \in \mathbb{R}^N$ span a subspace $\mathcal{S}$
- Find $\mathbf{w}$ such that $\mathbf{y} = (y(\mathbf{x}_1, \mathbf{w}), \ldots, y(\mathbf{x}_N, \mathbf{w}))^T \in \mathcal{S}$ is closest to $\mathbf{t}$.



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Sequential Learning - Stochastic Gradient Descent

- For large data sets, calculating the maximum likelihood parameters $\mathbf{w}_{ML}$ and β_{ML} may be costly.
- For real-time applications, never all data in memory.
- Use a sequential algorithms (online algorithm).
- If the error function is a sum over data points $E = \sum_n E_n$, then
  1. initialise $\mathbf{w}^{(0)}$ to some starting value
  2. update the parameter vector at iteration $\tau + 1$ by

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n,$$

where E_n is the error function after presenting the nth data set, and η is the learning rate.

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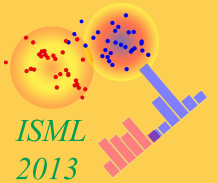

Sequential Learning - Stochastic Gradient Descent

- For the sum-of-squares error function, stochastic gradient descent results in

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \left(t_n - \mathbf{w}^{(\tau)T} \phi(\mathbf{x}_n) \right) \phi(\mathbf{x}_n)$$

- The value for the learning rate must be chosen carefully. A too large learning rate may prevent the algorithm from converging. A too small learning rate does follow the data too slowly.

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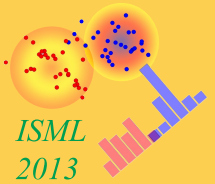

Regularized Least Squares

- Add regularisation in order to prevent overfitting

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

  with regularisation coefficient λ.
- Simple quadratic regulariser

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

- Maximum likelihood solution

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

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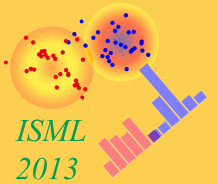
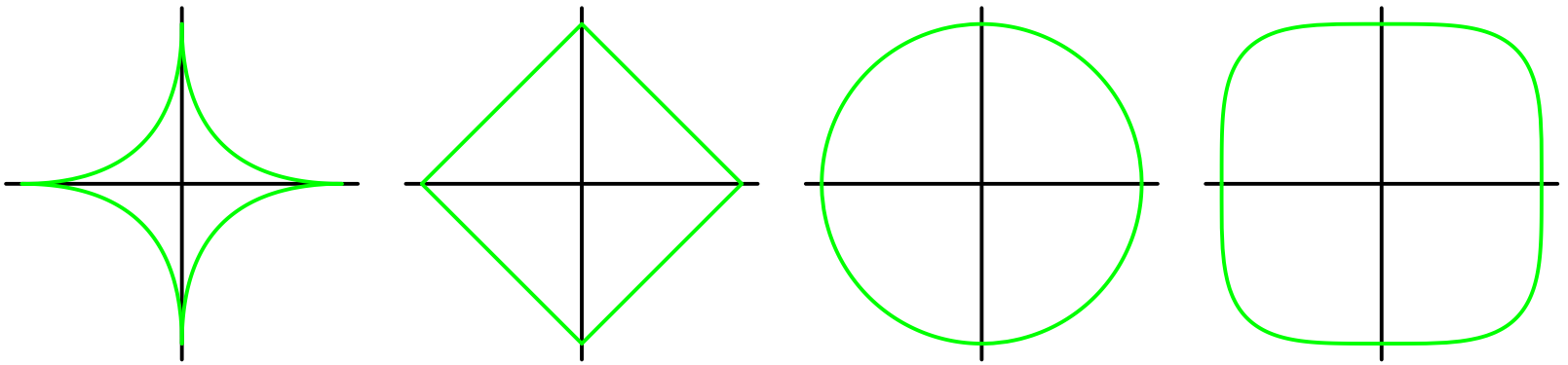


Regularized Least Squares

- More general regulariser

$$E_W(\mathbf{w}) = \frac{1}{2}\sum_{j=1}^{M}|w_j|^q$$

- $q = 1$ (lasso) leads to a sparse model if λ large enough.



q = 2 is usual, because each direction of w has no disparity

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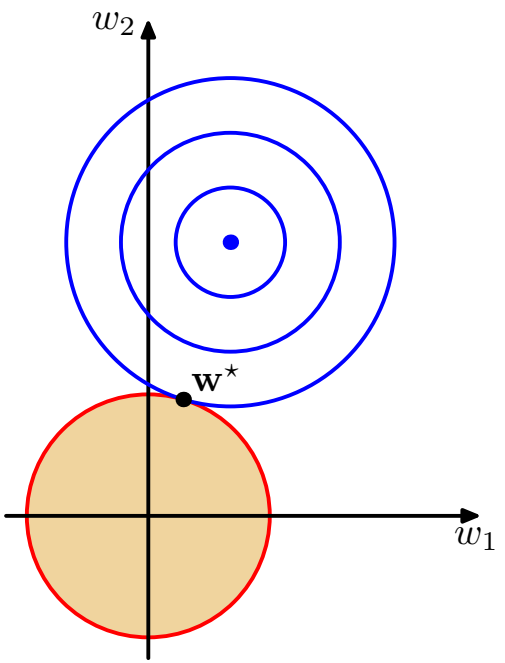
Comparison of Quadratic and Lasso Regulariser

Assume a sufficiently large regularisation coefficient λ.

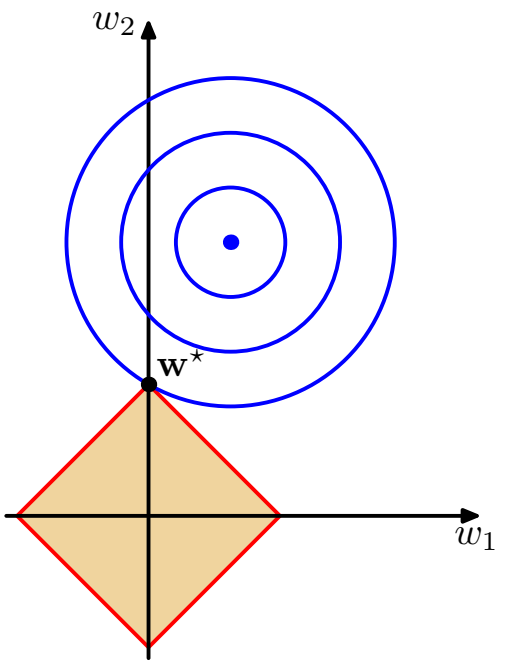
Quadratic regulariser

$$\frac{1}{2}\sum_{j=1}^{M} w_j^2$$



Lasso regulariser

$$\frac{1}{2}\sum_{j=1}^{M} |w_j|$$



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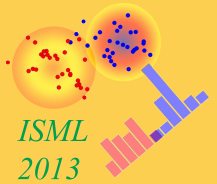

Multiple Outputs

- More than 1 target variable per data point.
- $\mathbf{y}$ becomes a vector instead of a scalar. Each dimension can be treated with a different set of basis functions (and that may be necessary if the data in the different target dimensions represent very different types of information.)
- Here we restrict ourselves to the SAME basis functions

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

  where $\mathbf{y}$ is a K-dimensional column vector, $\mathbf{W}^T$ is an $M \times K$ matrix of model parameters, and $\boldsymbol{\phi}(\mathbf{x}) = (\phi_0(\mathbf{x}), \ldots, \phi_{M-1}(\mathbf{x}), \phi_0(\mathbf{x}) = 1$, as before.
- Define target matrix $\mathbf{T}$ containing the target vector $\mathbf{t}_n^T$ in the n^{th} row.

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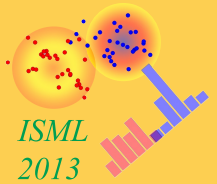

Multiple Outputs

- Suppose the conditional distribution of the target vector is an isotropic Gaussian of the form

$$p(\mathbf{t} \mid \mathbf{x}, \mathbf{W}, \beta) = \mathcal{N}(\mathbf{t} \mid \mathbf{W}^T \boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\mathbf{I}).$$

- The log likelihood is then

$$\begin{aligned}\ln p(\mathbf{T} \mid \mathbf{X}, \mathbf{W}, \beta) &= \sum_{n=1}^{N} \ln \mathcal{N}(\mathbf{t}_n \mid \mathbf{W}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1} VI) \\ &= \frac{NK}{2} \ln\left(\frac{\beta}{2\pi}\right) - \frac{\beta}{2} \sum_{n=1}^{N} \|\mathbf{t}_n - \mathbf{W}^T \boldsymbol{\phi}(\mathbf{x}_n)\|^2\end{aligned}$$

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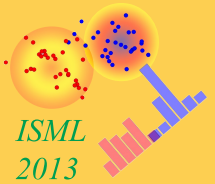

Multiple Outputs

- Maximisation with respect to $\mathbf{W}$ results in

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

- For each target variable $\mathbf{t}_k$, we get

$$\mathbf{w}_k = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{t}_k = \mathbf{\Phi}^\dagger\mathbf{t}_k.$$

- The solution between the different target variables decouples.
- Holds also for a general Gaussian noise distribution with arbitrary covariance matrix.
- Why? $\mathbf{W}$ defines the mean of the Gaussian noise distribution. And the maximum likelihood solution for the mean of a multivariate Gaussian is independent of the covariance.

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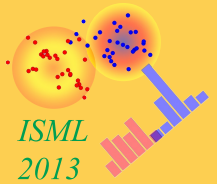

Loss Function for Regression

- Over-fitting results from a large number of basis functions and a relatively small training set.
- Regularisation can prevent overfitting, but how to find the correct value for the regularisation constant λ ?
- Frequentists viewpoint of the model complexity is the bias-variance trade-off.

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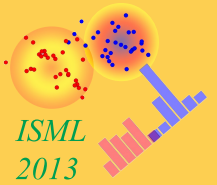

Loss Function for Regression

- Choose an estimator $y(\mathbf{x})$ to estimate the target value t for each input $\mathbf{x}$.
- Choose a loss function $L(t, y(\mathbf{x}))$ which measures the difference between the target t and the estimate $y(\mathbf{x})$.
- The expected loss is then

$$\mathbb{E}[L] = \int \int L(t, y(\mathbf{x}))\, p(\mathbf{x}, t)\, \mathrm{d}\mathbf{x}\, \mathrm{d}t$$

- Common choice: Squared Loss

$$L(t, y(\mathbf{x})) = \{y(\mathbf{x}) - t\}^2 .$$

- Expected loss for squared loss function

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

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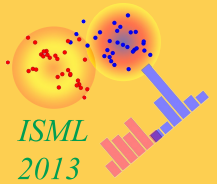


Loss Function for Regression

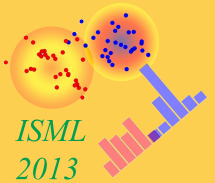
- Expected loss for squared loss function

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

- Minimise $\mathbb{E}[L]$ by choosing the regression function

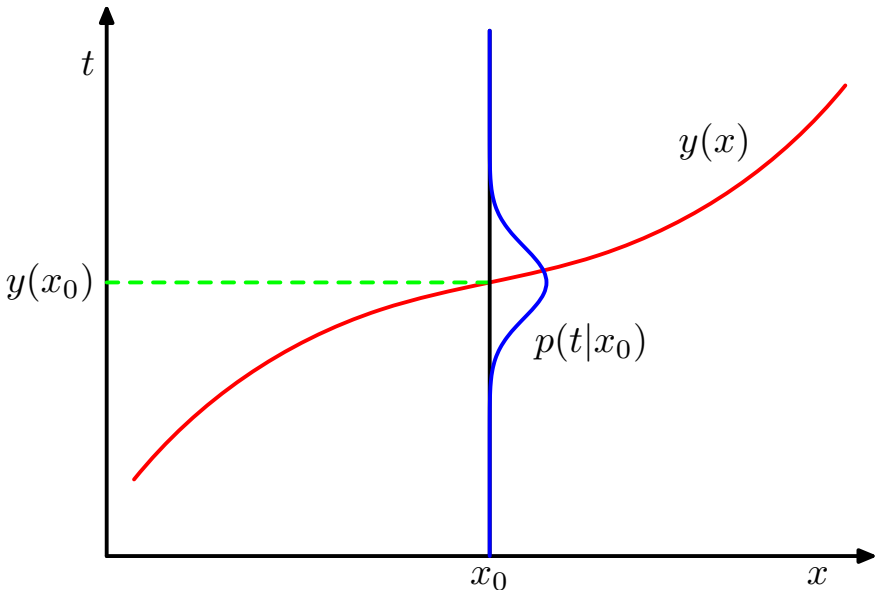
$$y(\mathbf{x}) = \frac{\int t \, p(\mathbf{x}, t) \, \mathrm{d}t}{p(\mathbf{x})} = \int t \, p(t \,|\, \mathbf{x}) \, \mathrm{d}t = \mathbb{E}_t[t \,|\, \mathbf{x}]$$

(use calculus of variations to derive this result).



Loss Function for Regression

- The regression function which minimises the expected squared loss, is given by the mean of the conditional distribution $p(t \mid \mathbf{x})$.



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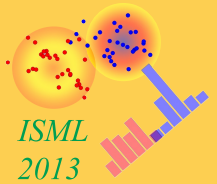

Loss Function for Regression

- Analyse the expected loss

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

- Rewrite the squared loss

$$\begin{aligned}\{y(\mathbf{x}) - t\}^2 &= \{y(\mathbf{x}) - \mathbb{E}[t \mid \mathbf{x}] + \mathbb{E}[t \mid \mathbf{x}] - t\}^2 \\ &= \{y(\mathbf{x}) - \mathbb{E}[t \mid \mathbf{x}]\}^2 + \{\mathbb{E}[t \mid \mathbf{x}] - t\}^2 \\ &\quad + 2\{y(\mathbf{x}) - \mathbb{E}[t \mid \mathbf{x}]\}\{\mathbb{E}[t \mid \mathbf{x}] - t\}\end{aligned}$$

- Claim

$$\int \int \{y(\mathbf{x}) - \mathbb{E}[t \mid \mathbf{x}]\}\{\mathbb{E}[t \mid \mathbf{x}] - t\} p(\mathbf{x}, t)\, \mathrm{d}\mathbf{x}\, \mathrm{d}t = 0.$$

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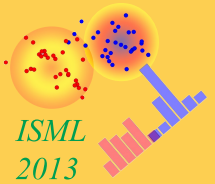

Loss Function for Regression

- Claim

$$\int \int \{y(\mathbf{x}) - \mathbb{E}[t \mid \mathbf{x}]\} \{\mathbb{E}[t \mid \mathbf{x}] - t\} p(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t = 0.$$

- Seperate functions depending on t from function depending on $\mathbf{x}$

$$\int \{y(\mathbf{x}) - \mathbb{E}[t \mid \mathbf{x}]\} \left(\int \{\mathbb{E}[t \mid \mathbf{x}] - t\} p(\mathbf{x}, t) \, \mathrm{d}t \right) \mathrm{d}\mathbf{x}$$

- Calculate the integral over t

$$\begin{aligned} \int \{\mathbb{E}[t \mid \mathbf{x}] - t\} p(\mathbf{x}, t) \, \mathrm{d}t &= \mathbb{E}[t \mid \mathbf{x}] p(\mathbf{x}) - p(\mathbf{x}) \int \frac{t \, p(\mathbf{x}, t)}{p(\mathbf{x})} \, \mathrm{d}t \\ &= \mathbb{E}[t \mid \mathbf{x}] p(\mathbf{x}) - p(\mathbf{x}) \mathbb{E}[t \mid \mathbf{x}] \\ &= 0 \end{aligned}$$

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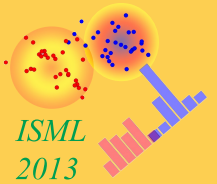

Loss Function for Regression

- The expected loss is now

$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - \mathbb{E}[t \mid \mathbf{x}]\}^2 p(\mathbf{x})\, d\mathbf{x} + \int \mathrm{var}[t \mid \mathbf{x}]\, p(\mathbf{x})\, d\mathbf{x}$$

- Minimise first term by choosing appropriate $y(\mathbf{x})$.
- Second term represents the intrinsic variability of the target data (can be regarded as noise). Independent of the choice $y(\mathbf{x})$, can not be reduced by learning a better $y(\mathbf{x})$.

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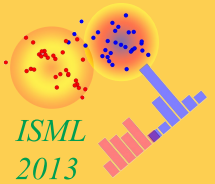

The Bias-Variance Decomposition

- Consider now the dependency on the data set $\mathcal{D}$.
- Prediction function now $y(\mathbf{x}; \mathcal{D})$.
- Consider again squared loss for which the optimal prediction is given by the conditional expectation $h(\mathbf{x})$

$$h(\mathbf{x}) = \mathbb{E}[t \mid \mathbf{x}] = \int t\, p(t \mid \mathbf{x})\, \mathrm{d}t.$$

- BUT: we can not know $h(x)$ exactly, as we would need an infinite number of training data to learn it accurately.
- Evaluate performance of algorithm by taking the expectation $\mathbb{E}_{\mathcal{D}}[L]$ over all data sets $\mathcal{D}$

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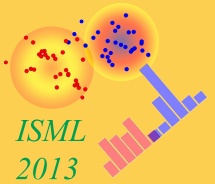


The Bias-Variance Decomposition

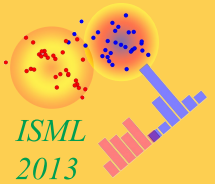
- Taking the expectation over all data sets $\mathcal{D}$

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

- Again, add and subtract the expectation $\mathbb{E}_{\mathcal{D}}\left[y(\mathbf{x};\mathcal{D})\right]$

$$\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2 = \{\, y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\mathbf{x};\mathcal{D})\right] + \mathbb{E}_{\mathcal{D}}\left[y(\mathbf{x};\mathcal{D})\right] - h(\mathbf{x})\}^2$$

and show that the mixed term does vanish under the expectation $\mathbb{E}_{\mathcal{D}}\left[\ldots\right]$.



The Bias-Variance Decomposition

- Expected loss $\mathbb{E}_{\mathcal{D}}[L]$ over all data sets $\mathcal{D}$

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}.$$

where

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

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

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

- squared bias : how much does the average prediction over all data sets differ from the desired regression function ?
- variance : how much do solutions for individual data sets vary around their average ?

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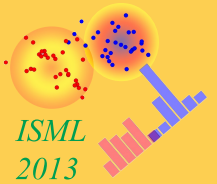
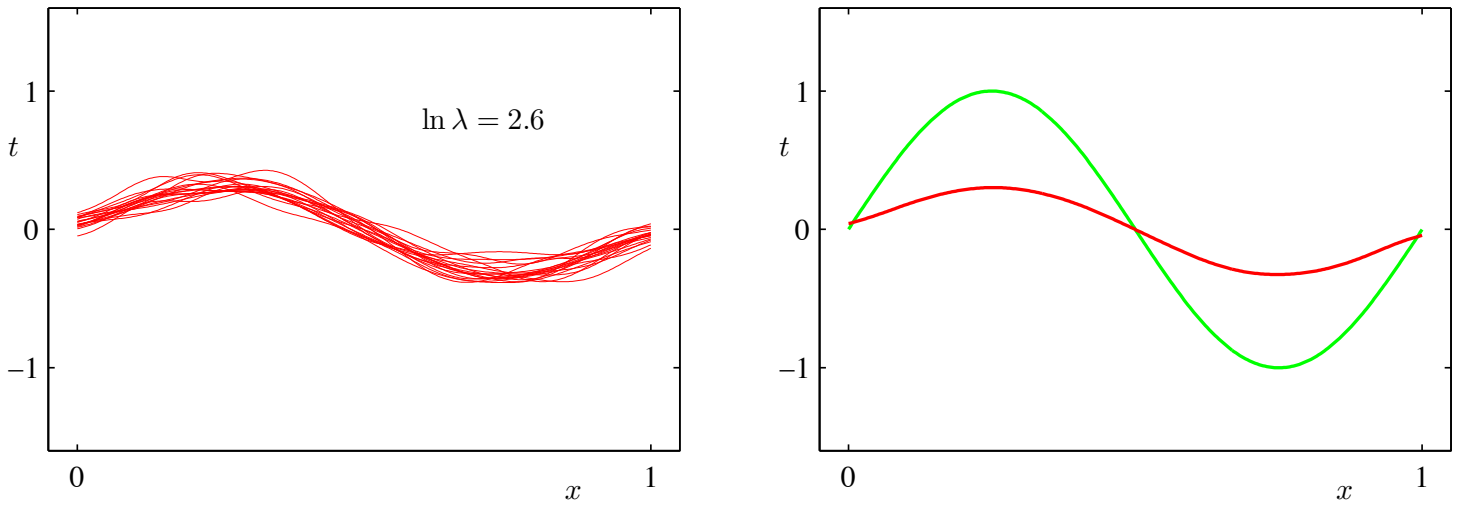


The Bias-Variance Decomposition

Dependence of bias and variance on the model complexity



Left: Result of fitting the model to 100 data sets, only 25 shown.
Right: Average of the 100 fits in red, the sinusoidal function from where the data were created in green.

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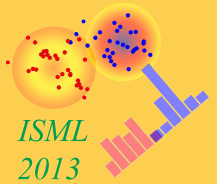

The Bias-Variance Decomposition

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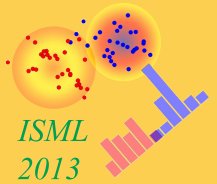
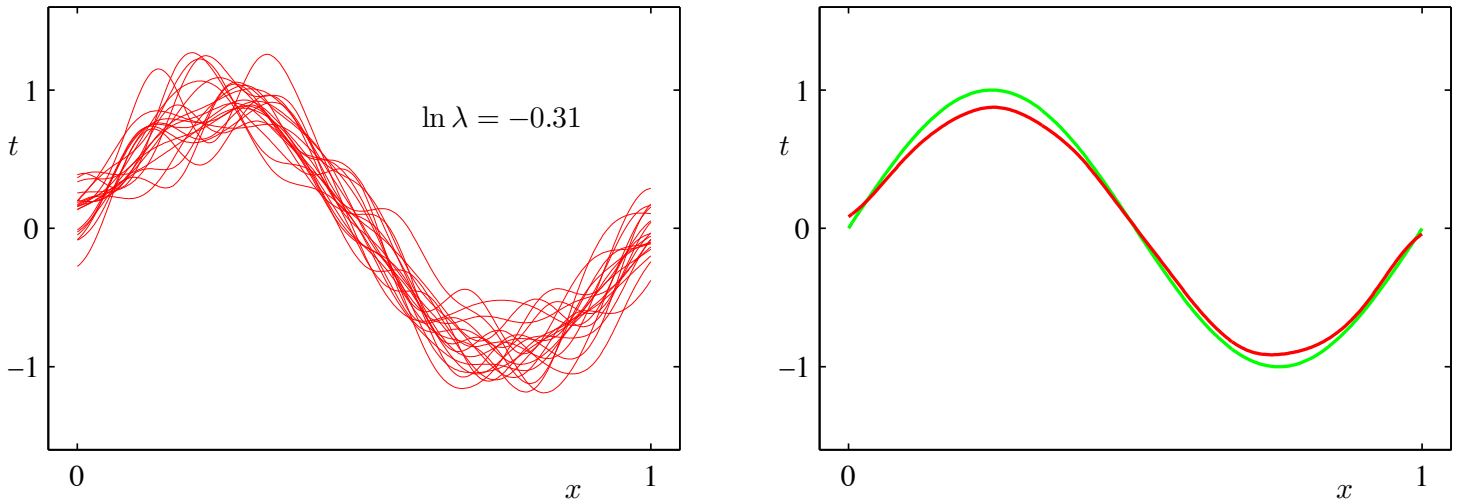


Dependence of bias and variance on the model complexity



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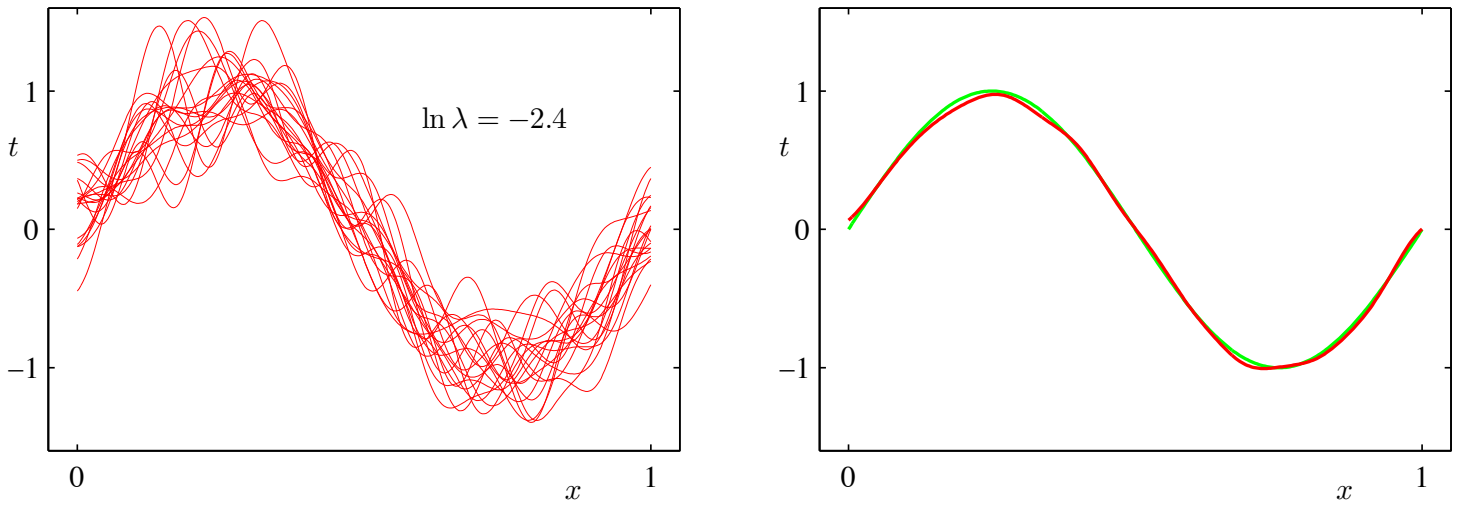
The Bias-Variance Decomposition

Dependence of bias and variance on the model complexity



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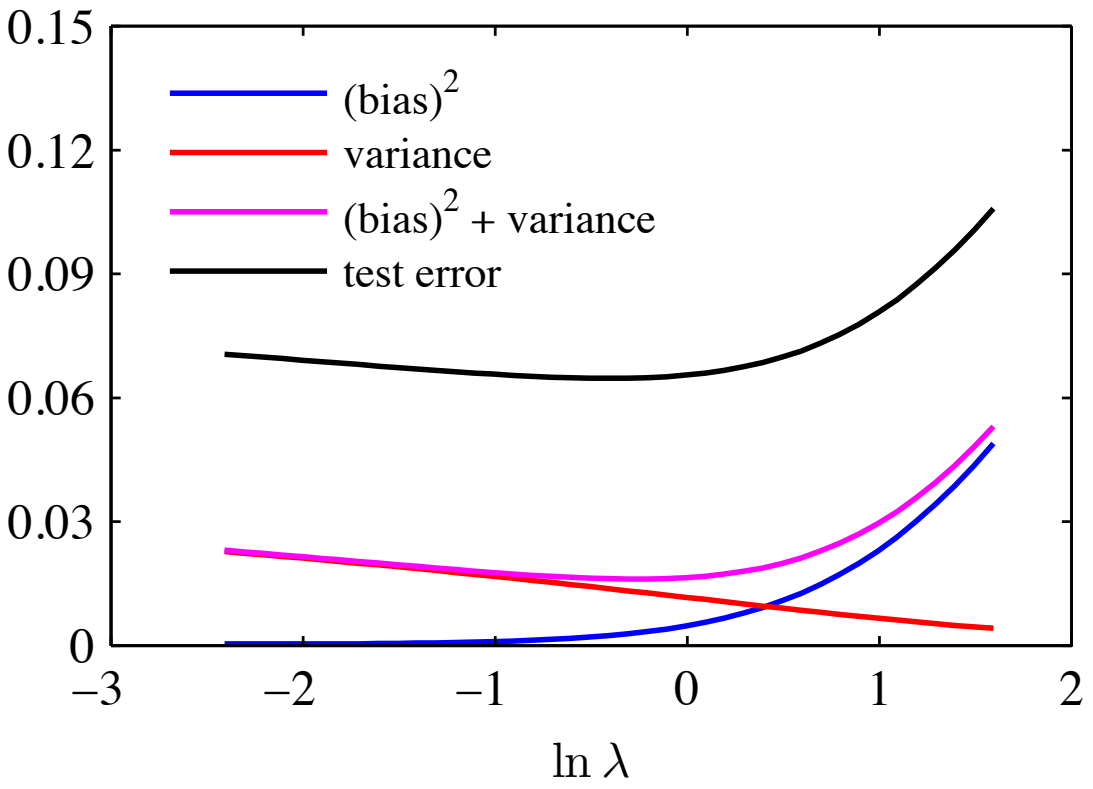
The Bias-Variance Decomposition

- Squared bias, variance, their sum, and test data
- The minimum for $(\text{bias})^2 + \text{variance}$ occurs close to the value that gives the minimum error



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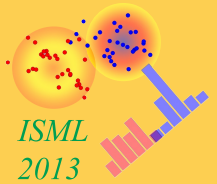

The Bias-Variance Decomposition

- Tradeoff between bias and variance
  - simple models have high bias and low variance
  - complex models have low bias and high variance
- The sum of bias and variance has a minimum at some model complexity.
- The bias-variance decomposition needs many data sets, which are not always available.

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