Statistical Machine Learning

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

Outlines

Part III

Linear Regression

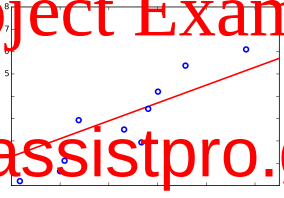
$N = 10$

$\mathbf{x} \equiv (x_1, \dots, x_N)^T$

$\mathbf{t}$

x_i

t_i



- Predictor $y(x, \mathbf{w})$?
- Performance measure?
- Optimal solution w^*?
- Recall: projection, inverse

Probabilities, Losses

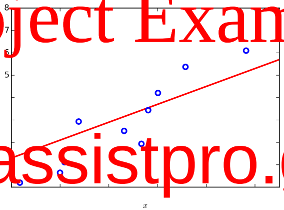
- Ga
- Ba
- Exp

Linear Curve Fitting - Least Squares

$$N = 10$$

$$\mathbf{x} \equiv (x_1, \ldots, x_N)^T$$

$$\mathbf{t} \equiv (t_1, \ldots, t_N)^T$$



$y(x,$

$$X \equiv [\mathbf{x} \quad 1]$$

$$w^* = (X^T X)^{-1} X^T \mathbf{t}$$

We assume

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

Curve fitting - revisited

- *a priori* belief about the parameter $\mathbf{w}$ captured in the prior probability $p(\mathbf{w})$
- obs
- cal
  obs

$$\overline{}$$
$$p(\mathcal{D})$$

- $p(\mathcal{D}\,|\,\mathbf{w})$ as a function of $\mathbf{w}$: likelihood fun
- likelihood expresses how probable the data ar different values of $\mathbf{w}$ — it is not a probability d respect $\mathbf{w}$ (but it is with respect to $\mathcal{D}$; prove it)

- Consider the linear regression problem, where we have random variables $\mathbf{x}_n$ and t_n.
- We
- We

For a given θ the density defines the probab observing $t_n|\mathbf{x}_n$.

- We are interested in finding θ that maxi probability (called the likelihood) of the data.

Likelihood function $p(\mathcal{D} \mid \mathbf{w})$

Frequentist Approach

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- v
  some 'estimator'
- error bars on the estimated $\mathbf{w}$ obtained from the distribution of possible data sets $\mathcal{D}$

Bayesian Approach

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- par
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  distr

Frequentist Estimator - Maximum Likelihood

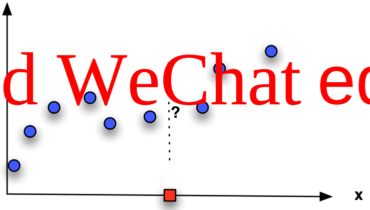
- choose $\mathbf{w}$ for which the likelihood $p(\mathcal{D} \mid \mathbf{w})$ (the probability of the observed data) is maximal
- the most common heuristic for learning a single fixed $\mathbf{w}$
- equ
  fun
- log i
- maximising the likelihood $\iff$ minimi
- Example: Fair-looking coin is tossed three tim
  landing on heads.
- Maximum likelihood estimate of the probability of landing heads will give 1.

Bayesian Approach

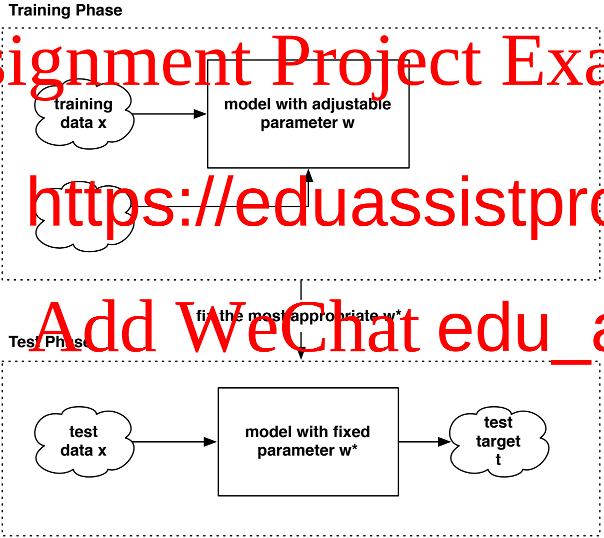
- including prior knowledge easy (via prior $\mathbf{w}$)
- subjective choice of prior, allows better results by incorporating domain knowledge
- sometimes choice of prior motivated by convinient mathematical form
- prio
- nee
  -
  - advances in approximation schemes (Vari Expectation Propagation)
- there is no true $\mathbf{w}$.

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 .
- Exa

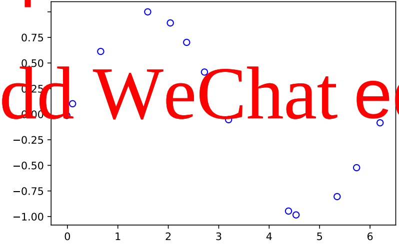


Supervised Learning: (non-Bayesian) Point Estimate



Why Linear Regression?

- Analytic solution when minimising sum of squared errors
- Well understood statistical behaviour
- Efficient algorithms exist for convex losses and regularizers
- But



Linear Basis Function Models

- Linear combination of fixed nonlinear basis functions

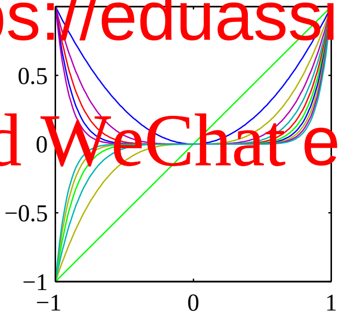
- parameter $\mathbf{w} = (w_0, \ldots, w_{M-1})$
- basis functions $\phi(\mathbf{x}) = (\phi_0(\mathbf{x}), \ldots, \phi_{M-}$
- convention $\phi_0(\mathbf{x}) = 1$
- w_0 is the bias parameter

Polynomial Basis Functions

- Scalar input variable x

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

- Limitation : Polynomials are global functions of the input variable x so the learned function will extrapolate poorly

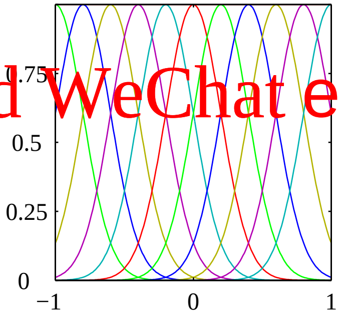


'Gaussian' Basis Functions

- 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 par
- We



Sigmoidal Basis Functions

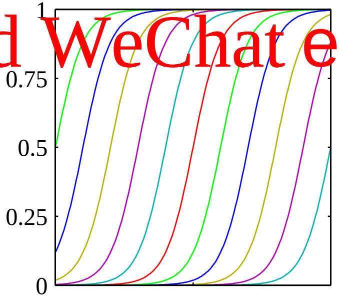
- Scalar input variable x

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

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

$$\frac{1}{\quad}$$

- $\sigma(a$ … tan



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).
- Spli
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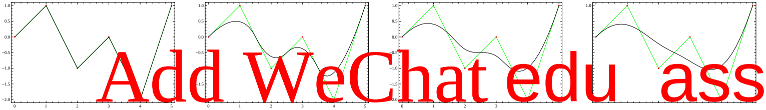

Linear Splines | Quadratic Splines | Cubic Splines | Splines

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

Maximum Likelihood and Least Squares

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

$$t = \underline{y(\mathbf{x}, \mathbf{w})} + \epsilon$$

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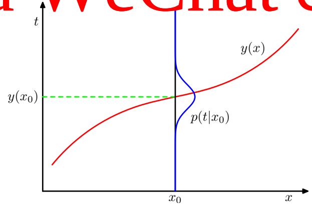
- Thus

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



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

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

- Now, a set of inputs $\mathbf{X}$ with corresponding target values $\mathbf{t}$.
- Ass
(i.i.
sa

$$p(\mathbf{t} \mid \mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n \mid y(\mathbf{x}_n$$

$$= \prod_{n=1}^{N} \mathcal{N}(t_n \mid \mathbf{w}^T \phi \quad n$$

- 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.

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

$$\ln p(\mathbf{t}\,|\,\mathbf{w},\beta) = \sum^{N} \ln \mathcal{N}(t_n\,|\,\mathbf{w}^T\phi(\mathbf{x}_n),\beta^{-1})$$

$$= \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) - \beta$$

where the sum-of-squares error function is

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

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

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

N

$-$ $-$

wh

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

- The log likelihood is now

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

- Fin
- The

$$\nabla_{\mathbf{w}} \ln \quad (\; | \quad , \beta) = \beta \mathbf{\Phi} \; (\qquad \mathbf{\Phi} \quad).$$

Setting the gradient to zero gives

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

- 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 $\mathbf{\Phi}$.

Maximum Likelihood and Least Squares

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

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

- Fin

results in

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

- 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 $\mathbf{w}$?

Sequential Learning - Stochastic Gradient Descent

- For large data sets, calculating the maximum likelihood parameters $\mathbf{w}_{ML}$ and β_{ML} may be costly.
- For
- Us
- If the
  then

  1. initialise $\mathbf{w}^{(0)}$ to some starting value
  2. update the parameter vector at iteration

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

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

Sequential Learning - Stochastic Gradient Descent

- For t des

- The value for the learning rate must be chosen ca too large learning rate may prevent the algorith converging. A too small learning rate does follo too slowly.

Regularized Least Squares

- Add regularisation in order to prevent overfitting

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

wit

- Sim

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

- Maximum likelihood solution

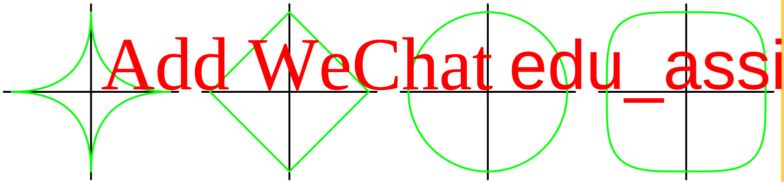
$$\mathbf{w} = \left(\lambda \mathbf{I} + \boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T\mathbf{t}$$

Regularized Least Squares

- More general regulariser

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

- $q =$



$q = 0.5$ $q = 1$ $q = 2$ $q = 4$

Lagrangian Dual View of the Regulariser

- By the Lagrange multiplier method, minimization of the regularized error function

$$\sum^{N} \qquad \sum^{M}$$

- is eq
sum-of-squares error,

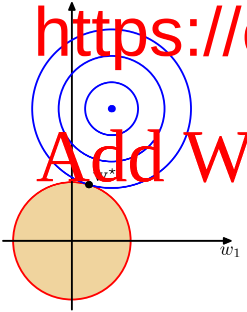
$$\frac{1}{2}\sum_{n=1}^{N}(t_n - \mathbf{w}^T\phi(\mathbf{x}_n))^2 \quad \text{subject to} \quad \sum_{j=1}$$

- This yields the figures on the next slide.

Comparison of Quadratic and Lasso Regulariser

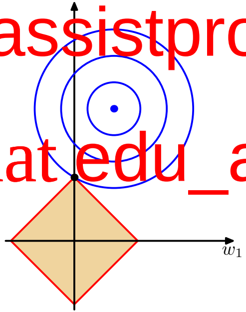
Quadratic regulariser

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



Lasso regulariser

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



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
dim
- Her

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

where $\mathbf{y}$ is a K-dimensional column vecto
matrix of model parameters, and
$\boldsymbol{\phi}(\mathbf{x}) = \Big(\phi_0(\mathbf{x}), \dots, \phi_{M-1}(\mathbf{x})\Big)$, with $\phi_0(\mathbf{x}) = 1$, as before.

- Define target matrix $\mathbf{T}$ containing the target vector $\mathbf{t}_n^T$ in the n^{th} row.

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

- Then

$$\ln p(\mathbf{T} \mid \mathbf{X}, \mathbf{W}, \beta) = \sum_{n=1}^{N} \ln \mathcal{N}(\mathbf{t}_n \mid \mathbf{W}^T \phi(\mathbf{x}$$

$$= \frac{NK}{2} \ln \left(\frac{\beta}{2\pi} \right) - \frac{\beta}{2}$$

Multiple Outputs

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

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

- For

- The
decouples.
- Holds also for a general Gaussian noise distrib
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.

Loss Function for Regression

- Ov
  and
- Re
  corr
- Frequentists viewpoint of the model complex
  bias-variance trade-off.

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
- Common choice: Squared Loss

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

- Expected loss for squared loss function

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

Loss Function for Regression

- Expected loss for squared loss function

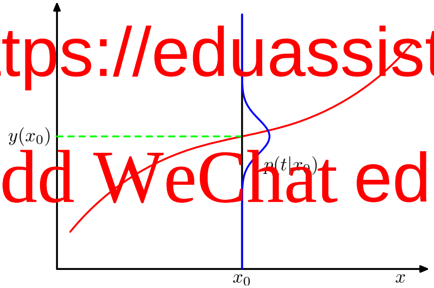
$$2$$

- Min

$$y(\mathbf{x}) = \frac{t\, p(\mathbf{x}, t)\, \mathrm{d}t}{p(\mathbf{x})} = \quad t\, p(t \mid \mathbf{x}$$

(calculus of variations is not required to derive th
we may work point-wise by fixing an $\mathbf{x}$
stationarity to solve for $y(\mathbf{x})$ — why is that sufficient?).

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



Analysing the Squared Loss (1)

- Analyse the expected loss

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

- Re

$$= \{y(\mathbf{x}) - \mathbb{E}[t \,|\, \mathbf{x}]\}^2 + \qquad {}^2$$

$$+ 2\{y(\mathbf{x}) - \mathbb{E}[t \,|\, \mathbf{x}]\}\{$$

- Claim

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

- Claim

$$\iint \{y(\mathbf{x}) - \mathbb{E}\left[t \,|\, \mathbf{x}\right]\}\{\mathbb{E}\left[t \,|\, \mathbf{x}\right] - t\}\, p(\mathbf{x}, t)\, \mathrm{d}\mathbf{x}\, \mathrm{d}t = 0$$

- Se
dep

- Calculate the integral over t

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

- The expected loss is now

$\mathbb{E}$

- Min
already).
- Second term represents the intrinsic variabilit
target data (can be regarded as noise). Indepe
choice $y(\mathbf{x})$, can not be reduced by learning a be

The Bias-Variance Decomposition (1)

- Consider again squared loss for which the optimal prediction is given by the conditional expectation $h(x)$

- Sin (fini $\mathcal{D}$
- $\mathcal{D}$ is a finite sample from the unknown joint
- Notate the dependency of the learned function by $y(\mathbf{x}; \mathcal{D})$.
- Evaluate performance of algorithm by taking the expectation $\mathbb{E}_{\mathcal{D}}[L]$ over all data sets $\mathcal{D}$

The Bias-Variance Decomposition (2)

- Taking the expectation over data sets $\mathcal{D}$, using Eqn 1, and interchanging the order of expectations for the first term:

$$2$$

- Again, add and subtract the expectation

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

and show that the mixed term vanishes under the expectation $\mathbb{E}_{\mathcal{D}}$.

The Bias-Variance Decomposition (3)

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

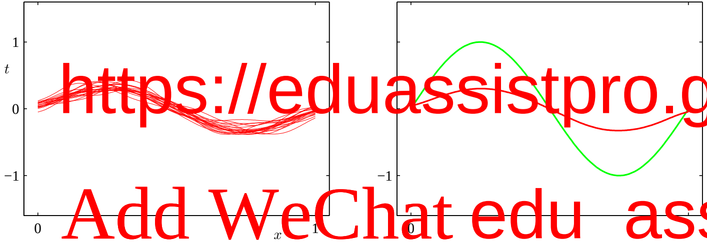
$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}.$$

where

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

- $(\text{bias})^2$: How accurate is a model across differe sets? (How much does the average prediction over all data sets differ from the desired regression function ?)
- variance : How sensitive is the model to small changes in the training set? (How much do solutions for individual data sets vary around their average ?

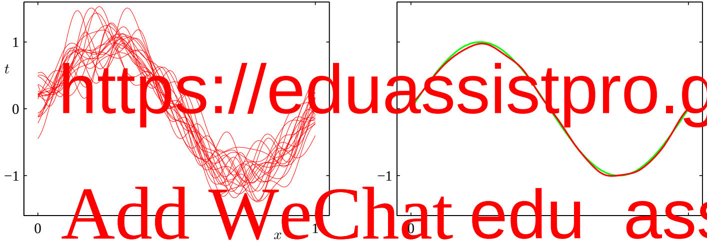
- Simple models have low variance and high bias.



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

The Bias-Variance Decomposition

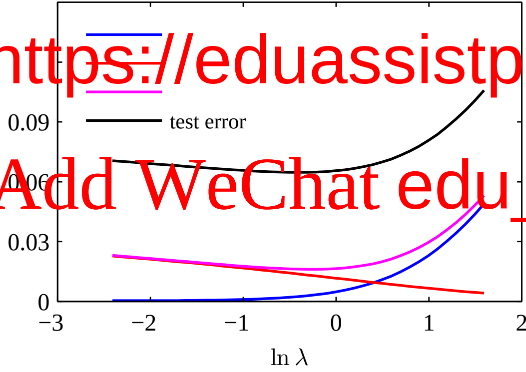
Complex models have high variance and low bias



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

The Bias-Variance Decomposition

- Dependence of bias and variance on the model complexity
- 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



Unbiased Estimators

- You may have encountered *unbiased estimators*
- Why guarantee zero bias? To quote the pioneer of Bayesian inference, Edwin Jaynes, from his book *Pro*

The Bias-Variance Decomposition

- Tradeoff between bias and variance
  - simple models have low variance and high bias
  - complex models have high variance and low bias
- The
  mo
- Exp

$$\text{expected loss} = (\text{bias})^2 + \text{varia}$$

- The noise comes from the data, and can not be re
  from the expected loss.
- To analyse the bias-variance decomposition : many data sets needed, which are not always available.