Introduction to Statistical Machine Learning

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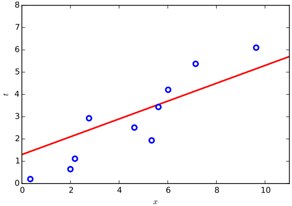
(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Part V

Linear Regression 1

Linear Regression

$$N = 10$$
$$\mathbf{x} \equiv (x_1, \dots, x_N)^T$$
$$\mathbf{t} \equiv (t_1, \dots, t_N)^T$$
$$x_i \in \mathbb{R} \quad i = 1,\dots, N$$
$$t_i \in \mathbb{R} \quad i = 1,\dots, N$$



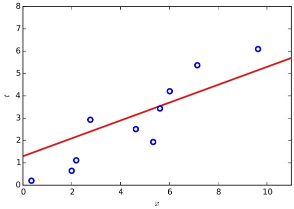
- Predictor $y(x, \mathbf{w})$?
- Performance measure?
- Optimal solution w^*?
- Recall: projection, inverse, eigenvalue decompostion

Probabilities, Losses

- Gaussian Distribution
- Bayes Rule
- Expected Loss
- Cross Validation

Linear Curve Fitting - Least Squares

$$N = 10$$
$$\mathbf{x} \equiv (x_1, \dots, x_N)^T$$
$$\mathbf{t} \equiv (t_1, \dots, t_N)^T$$
$$x_i \in \mathbb{R} \quad i = 1, \dots, N$$
$$t_i \in \mathbb{R} \quad i = 1, \dots, N$$
$$y(x, \mathbf{w}) = w_1 x + w_0$$
$$X \equiv [\mathbf{x} \quad 1]$$
$$w^* = (X^T X)^{-1} X^T \mathbf{t}$$



We assume

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

Curve fitting - revisited

- uncertainty about the parameter $\mathbf{w}$ captured in the prior probability $p(\mathbf{w})$
- observed data $\mathcal{D} = \{t_1, \dots, t_N\}$
- calculate the uncertainty in $\mathbf{w}$ after the data $\mathcal{D}$ have been observed

$$p(\mathbf{w} \,|\, \mathcal{D}) = \frac{p(\mathcal{D} \,|\, \mathbf{w}) p(\mathbf{w})}{p(\mathcal{D})}$$

- $p(\mathcal{D} \,|\, \mathbf{w})$ as a function of $\mathbf{w}$: likelihood function
- likelihood expresses how probable the data are for different values of $\mathbf{w}$
- not a probability function over $\mathbf{w}$

Maximum Likelihood

- Consider the linear regression problem, where we have random variables $\mathbf{x}_n$ and t_n.
- We assume a conditional model $t_n | \mathbf{x}_n$
- We propose a distribution, parameterized by θ

$$t_n | \mathbf{x}_n \sim \text{density}(\theta)$$

  For a given θ the density defines the probability of observing $t_n | \mathbf{x}_n$.
- We are interested in finding θ that maximises the probability (called the likelihood) of the data.

Likelihood Function - Frequentist versus Bayesian

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

Frequentist Approach

- $\mathbf{w}$ considered fixed parameter
- value defined by some 'estimator'
- error bars on the estimated $\mathbf{w}$ obtained from the distribution of possible data sets $\mathcal{D}$

Bayesian Approach

- only one single data set $\mathcal{D}$
- uncertainty in the parameters comes from a probability distribution over $\mathbf{w}$

Frequentist Estimator - Maximum Likelihood

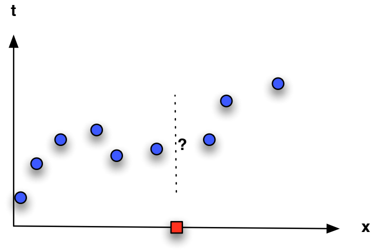
- choose $\mathbf{w}$ for which the likelihood $p(\mathcal{D} \mid \mathbf{w})$ is maximal
- choose $\mathbf{w}$ for which the probability of the observed data is maximal
- Machine Learning: error function is negative log of likelihood function
- log is a monoton function
- maximising the likelihood $\iff$ minimising the error
- Example: Fair-looking coin is tossed three times, always landing on heads.
- Maximum likelihood estimate of the probability of landing heads will give 1.

Bayesian Approach

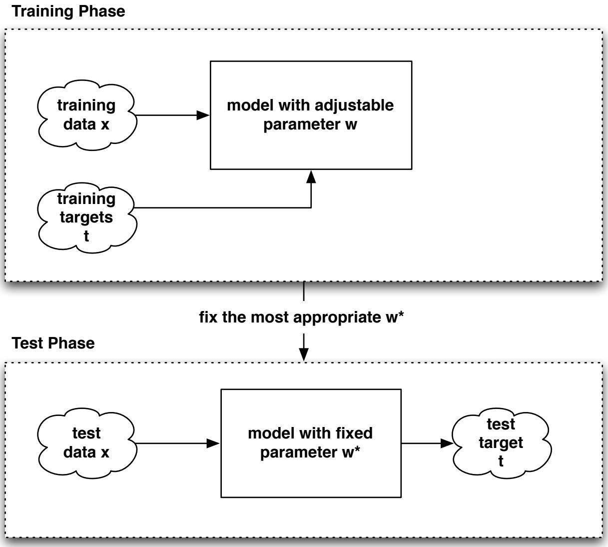
- including prior knowledge easy (via prior $\mathbf{w}$)
- BUT: if prior is badly chosen, can lead to bad results
- subjective choice of prior
- sometimes choice of prior motivated by convinient mathematical form
- need to sum/integrate over the whole parameter space
- advances in sampling (Markov Chain Monte Carlo methods)
- advances in approximation schemes (Variational Bayes, Expectation Propagation)

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).

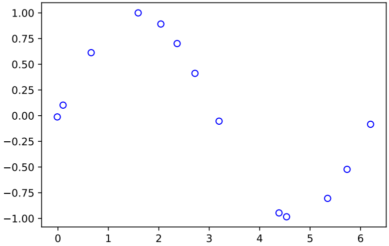


Supervised Learning



Why Linear Regression?

- Analytic solution when using least squares loss
- Well understood statistical behaviour
- Efficient algorithms exist for convex losses and regularizers
- But what if the relationship is non-linear?



Linear Basis Function Models

- Linear combination of fixed nonlinear basis functions

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

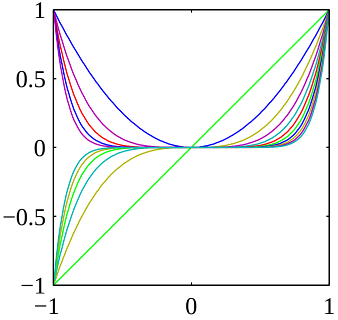
- parameter $\mathbf{w} = (w_0, \dots, w_{M-1})^T$
- basis functions $\boldsymbol{\phi}(\mathbf{x}) = (\phi_0(\mathbf{x}), \dots, \phi_{M-1}(\mathbf{x}))^T$
- convention $\phi_0(\mathbf{x}) = 1$
- w_0 is the bias parameter

Polynomial Basis Functions

- Scalar input variable x

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

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

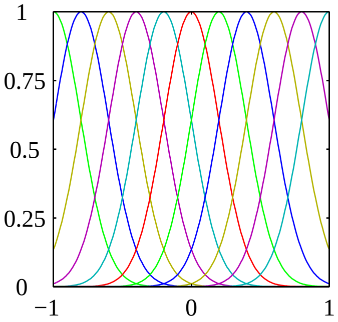


'Gaussian' Basis Functions

- 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.



Sigmoidal Basis Functions

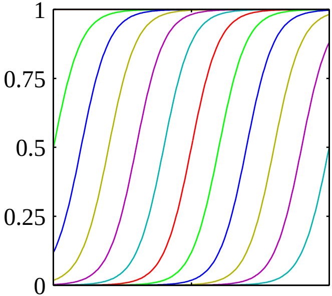
- Scalar input variable x

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

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

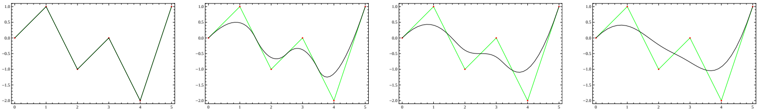
$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

- $\sigma(a)$ 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.

Maximum Likelihood and Least Squares

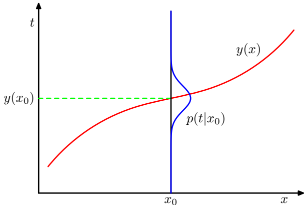
- No special assumption about the basis functions $\phi_j(\mathbf{x})$. In the simplest case, one can think of $\phi_j(\mathbf{x}) = x_j$, or $\boldsymbol{\phi}(\mathbf{x}) = \mathbf{x}$.
- Assume target t is given by

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

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

- Thus

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



Maximum Likelihood and Least Squares

- 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 $\mathbf{t}$.
- 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

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

- 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.

Maximum Likelihood and Least Squares

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

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

where the sum-of-squares error function is

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

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

Maximum Likelihood and Least Squares

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

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

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

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

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 $\ln p(\mathbf{t} \mid \mathbf{w}, \beta)$.
- The gradient with respect to $\mathbf{w}$ is

$$\nabla_{\mathbf{w}} \ln p(\mathbf{t} \mid \mathbf{w}, \beta) = \beta \mathbf{\Phi}^T (\mathbf{t} - \mathbf{\Phi w}).$$

  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

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

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

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

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 $\mathbf{w}$?

Sequential Learning - Stochastic Gradient Descent

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

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.

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

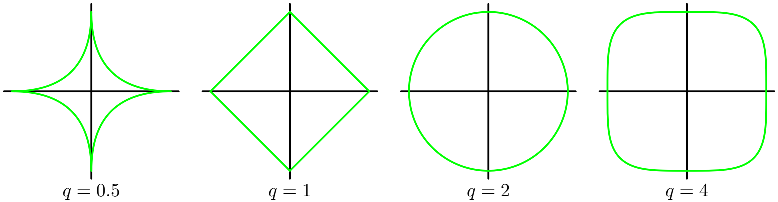
$$\mathbf{w} = \left(\lambda \mathbf{I} + \boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T\mathbf{t}$$

Regularized Least Squares

- More general regulariser

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

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

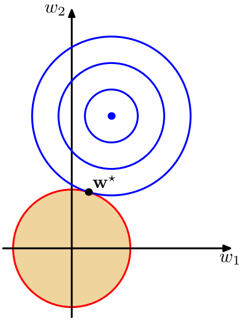


Comparison of Quadratic and Lasso Regulariser

Assume a sufficiently large regularisation coefficient λ.

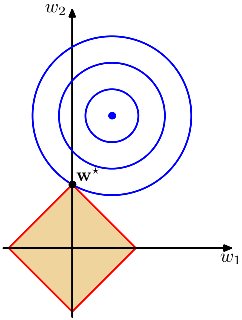
Quadratic regulariser

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



Lasso regulariser

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



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

Multiple Outputs

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

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

- The log likelihood is then

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

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.

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.

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

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

- Common choice: Squared Loss

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

- Expected loss for squared loss function

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

Loss Function for Regression

- Expected loss for squared loss function

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

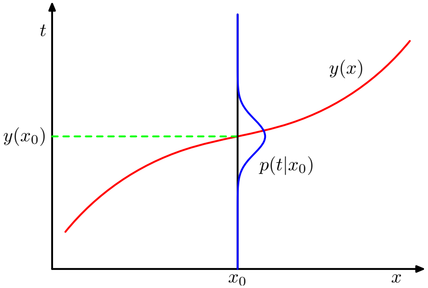
- Minimise $\mathbb{E}\left[L\right]$ by choosing the regression function

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

(use calculus of variations to derive this result ; alternatively work point-wise by fixing an $\mathbf{x}$ and using stationarity to solve for $y(\mathbf{x})$).

Loss Function for Regression

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



Loss Function for Regression

- Analyse the expected loss

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

- Rewrite the squared loss

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

- Claim

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

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

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

Loss Function for Regression

- The expected loss is now

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

- 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 $y(\mathbf{x})$.

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 $h(\mathbf{x})$

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

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

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

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

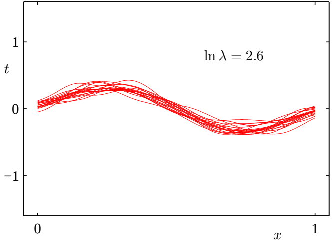
$$\text{variance} = \int \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right] p(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

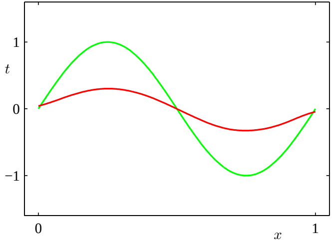
$$\text{noise} = \int\int \{h(\mathbf{x}) - t\}^2 \, p(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t.$$

- 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 ?
- squared bias : How accurate is a model across different training sets? (How much does the average prediction over all data sets differ from the desired regression function ?)

The Bias-Variance Decomposition

Simple models have low variance and high bias.

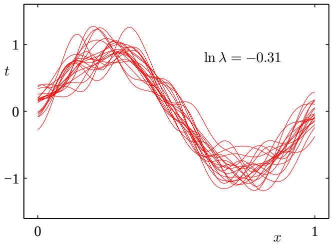


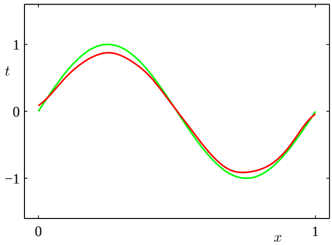


Left: Result of fitting the model to 100 data sets, only 25 shown.
Right: Average of the 100 fits in red, the sinusoidal function from where the data were created in green.

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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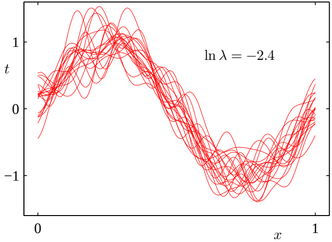
The Bias-Variance Decomposition

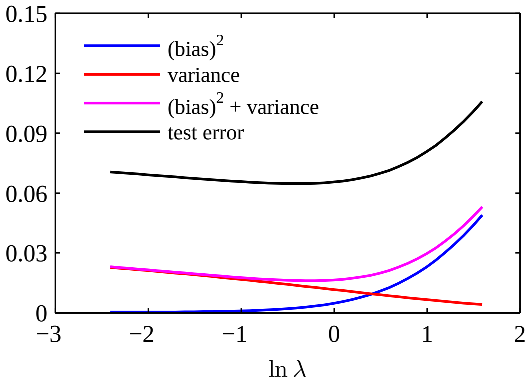
Complex models have high variance and low bias.



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.

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



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 sum of bias and variance has a minimum at a certain model complexity.
- Expected loss $\mathbb{E}_{\mathcal{D}}[L]$ over all data sets $\mathcal{D}$

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

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

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