



機械学習 Machine Learning

線形回帰モデル Linear Models for Regression

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線形回帰 Linear regression

訓練データ Training data 入力変数 Input variables: $\{\mathbf{x}_n\}$ $n = 1, \dots, N$
目標変数 Target variables: $\{t_n\}$

新しいデータ New data $\mathbf{x} \longrightarrow y(\mathbf{x}, \mathbf{w}) \Rightarrow t$ 予測 Prediction

訓練データより学習可能なパラメータ \mathbf{w}
Parameter that can be learned from
the training data

w_0, \dots, w_D に関する線形関数
A linear function of w_0, \dots, w_D

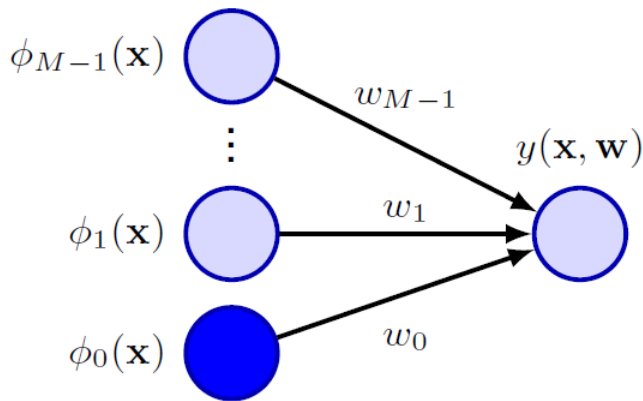
最もシンプルな回帰モデル
The simplest model for regression

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \dots + w_D x_D$$
$$\mathbf{x} = (x_1, \dots, x_D)^T \quad \mathbf{w} = (w_0, \dots, w_D)^T$$

線形回帰 Linear regression

基底関数 Basis functions

入力変数に関して非線形な関数の線形結合
Linear combinations of fixed nonlinear functions of the input variables



$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x})$$

$\phi_j(\mathbf{x})$ 基底関数 Basis functions

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

$\phi_0(\mathbf{x}) = 1$ w_0 バイアス Bias

$$\mathbf{w} = (w_0, \dots, w_{M-1})^T \quad \boldsymbol{\phi} = (\phi_0, \dots, \phi_{M-1})^T$$

線形回帰 Linear regression

基底関数 Basis functions

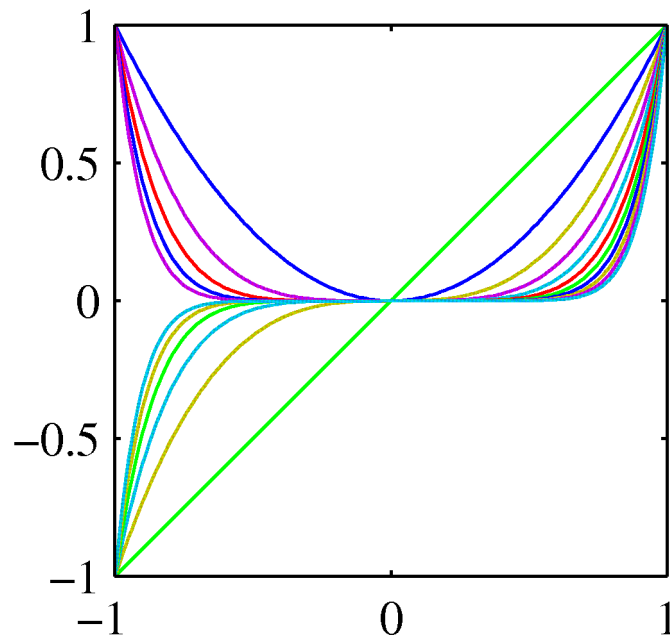
$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

基底関数の例

An example of the basis functions

多項式 Polynomial functions

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



線形回帰 Linear regression

基底関数 Basis functions

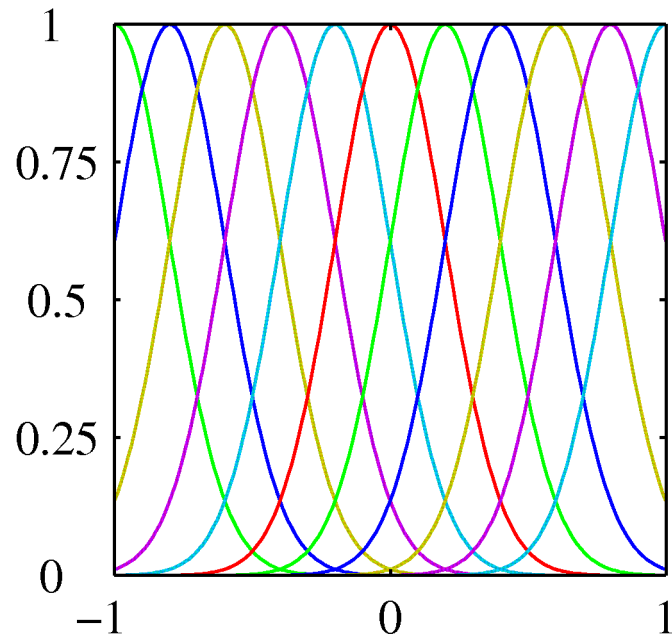
$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

基底関数の例

An example of the basis functions

ガウス基底関数 Gaussian basis functions

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



線形回帰 Linear regression

基底関数 Basis functions

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

基底関数の例

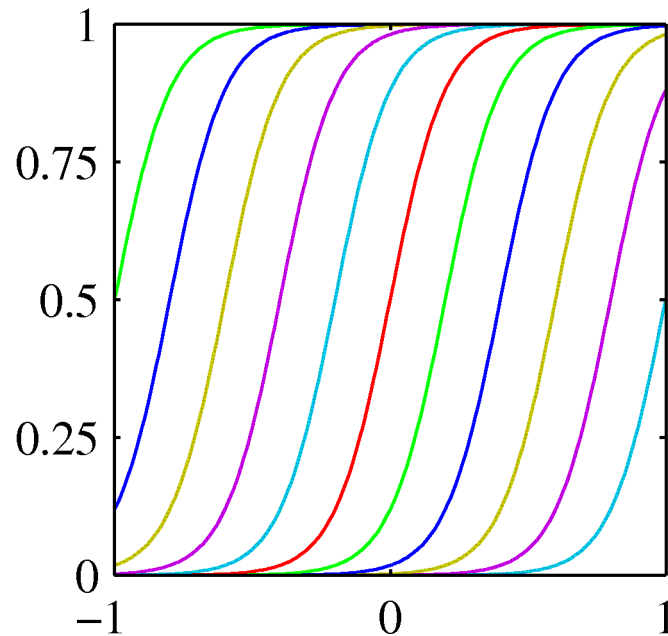
An example of the basis functions

シグモイド基底関数 Sigmoid basis functions

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

ロジスティックシグモイド関数
Logistic sigmoid function

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



線形回帰 Linear regression

尤度関数 Likelihood function

目標変数 t が決定論的な関数 $y(\mathbf{x}, \mathbf{w})$ と加法性のガウスノイズの和で与えられるとき
We assume that the target variable t is given by a deterministic function $y(\mathbf{x}, \mathbf{w})$ with additive Gaussian noise:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon \quad \text{ただし where } p(\epsilon|\sigma^2) = \mathcal{N}(\epsilon|0, \sigma^2)$$

$$\longrightarrow p(t|\mathbf{x}, \mathbf{w}, \sigma^2) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \sigma^2)$$

入力 Inputs: $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ 目標値 Target values: $\mathbf{t} = [t_1, \dots, t_N]^T$

尤度関数
Likelihood function

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2) = \prod_{n=1}^N \mathcal{N}(t_n|\mathbf{w}^T \phi(\mathbf{x}_n), \sigma^2)$$

線形回帰 Linear regression

尤度関数 Likelihood function

尤度関数の対数をとると

Taking the logarithm, we get

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

二乗和誤差関数

Sum-of-squares error

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

線形回帰 Linear regression

最尤推定 Maximum likelihood

$$\nabla_{\mathbf{w}} \ln p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2) = \frac{1}{\sigma^2} \sum_{n=1}^N \{t_n - \mathbf{w}^T \phi(\mathbf{x}_n)\} \phi(\mathbf{x}_n)^T$$

対数尤度関数の \mathbf{w} についての勾配を0とおけば

Setting the gradient of the log likelihood function with respect to \mathbf{w} to zero gives

$$0 = \sum_{n=1}^N t_n \phi(\mathbf{x}_n)^T - \mathbf{w}^T \left(\sum_{n=1}^N \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right)$$

$$\Rightarrow \mathbf{w}_{\text{ML}} = \underbrace{(\Phi^T \Phi)^{-1}}_{\rightarrow \Phi^\dagger} \Phi^T \mathbf{t} \quad \text{ただし } \mathbf{t} = [t_1, \dots, t_N]^T$$

where

ムーア-ペンローズの擬似逆行列
Moore-Penrose pseudo-inverse matrix

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

線形回帰 Linear regression

最尤推定 Maximum likelihood

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

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

w_0 について最大化すると

Maximizing with respect to w_0 , we see that

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

$$\bar{t} = \frac{1}{N} \sum_{n=1}^N t_n$$

$$\overline{\phi_j} = \frac{1}{N} \sum_{n=1}^N \phi_j(\mathbf{x}_n)$$

線形回帰 Linear regression

最尤推定 Maximum likelihood

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

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

σ^2 について最大化すると

Maximizing with respect to σ^2 , we see that

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

線形回帰 Linear regression

最小二乗法の幾何学 Geometry of least squares

$$\mathbf{y} = \Phi \mathbf{w}_{\text{ML}} = [\varphi_1, \dots, \varphi_M] \mathbf{w}_{\text{ML}}.$$

$$\mathbf{y} \in \mathcal{S} \subseteq \mathcal{T}$$

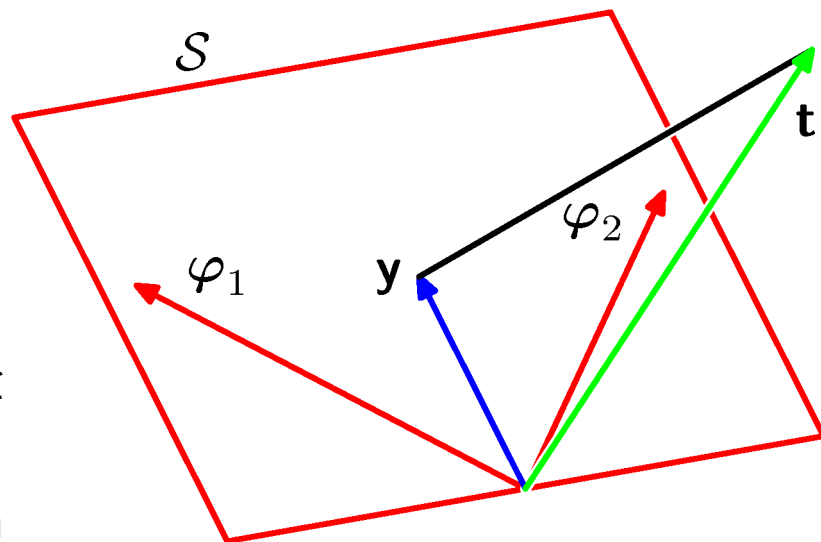
M 次元
 M dimensional

$$\mathbf{t} \in \mathcal{T}$$

N 次元
 N dimensional

\mathbf{w}_{ML} は \mathbf{t} と \mathbf{y} の二乗ユークリッド距離を最小化する.

\mathbf{w}_{ML} minimizes the squared Euclidean distance between \mathbf{t} and \mathbf{y} .



線形回帰 Linear regression

逐次学習 Sequential learning

逐次学習 Sequential learning

データ点を一度に1つだけ用いてモデルのパラメータを順次更新する。

Data points are considered one at a time and the model parameters are updated after each such presentation.

確率的勾配降下法 Stochastic gradient descent

$$\begin{aligned}\mathbf{w}^{(\tau+1)} &= \mathbf{w}^{(\tau)} - \eta \nabla E_n \\ &= \mathbf{w}^{(\tau)} + \eta (t_n - \mathbf{w}^{(\tau)\top} \phi(\mathbf{x}_n)) \phi(\mathbf{x}_n).\end{aligned}$$

$$E = \sum_n E_n$$

$$E_n = \frac{1}{2} (t_n - \mathbf{w}^{(\tau)\top} \phi_n)^2$$

線形回帰 Linear regression

正則化最小二乗法 Regularized least squares

以下の誤差関数を考える Consider the error function:

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

データに依存する誤差 Data-dependent error	正則化項 Regularization term	λ 正則化定数 Regularization coefficient
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二乗和誤差関数と重みベクトルの二乗和を用いるときは
With the sum-of-squares error function and
the sum of the squares of the weight vector elements, we get

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

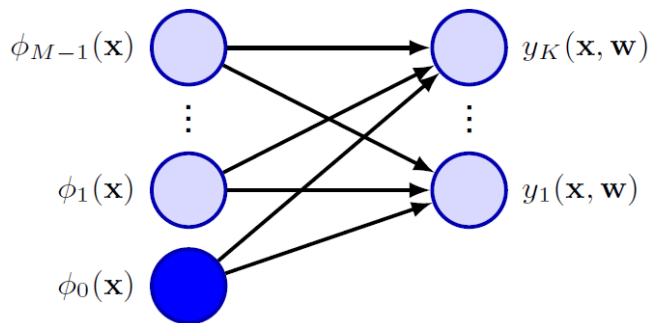
これは次のとき最小 which is minimized by $\mathbf{w} = \left(\lambda \mathbf{I} + \Phi^T \Phi \right)^{-1} \Phi^T \mathbf{t}$.

線形回帰 Linear regression

出力変数が多次元の場合 Multiple outputs

$K > 1$ 次元の目標変数を予測したい場合

When we wish to predict $K > 1$ target variables:



$$p(\mathbf{t}|\mathbf{x}, \mathbf{W}, \sigma^2) = \mathcal{N}(\mathbf{t}|\mathbf{W}^T \phi(\mathbf{x}), \sigma^2 \mathbf{I}) \quad \mathbf{t} = (t_1, \dots, t_K)^T$$

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

対数尤度関数 Log likelihood function

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

入力 Inputs:

$$\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$$

目標値 Target values:

$$\mathbf{T} = [\mathbf{t}_1, \dots, \mathbf{t}_N]^T$$

線形回帰 Linear regression

出力変数が多次元の場合 Multiple outputs

尤度を最大化する \mathbf{W} は

Maximizing the likelihood with respect to \mathbf{W} , we obtain

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

個々の目標変数 \mathbf{t}_k について評価すれば

If we consider a single target variable \mathbf{t}_k , we see that

$$\mathbf{w}_k = \left(\Phi^T \Phi \right)^{-1} \Phi^T \mathbf{t}_k = \Phi^\dagger \mathbf{t}_k \quad \mathbf{t}_k = [t_{1k}, \dots, t_{Nk}]^T$$

決定理論 Decision theory

推論段階 Inference stage

$p(t|\mathbf{x})$ を求める.

Determine $p(t|\mathbf{x})$.

例 e.g. $p(t|\mathbf{x}, \mathbf{w}_{\text{ML}}, \sigma_{\text{ML}}^2) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}_{\text{ML}}), \sigma_{\text{ML}}^2)$

決定段階 Decision stage

ある \mathbf{x} に対する t として最適な予測 $f(\mathbf{x})$ を行う.

For given \mathbf{x} , make optimal prediction $f(\mathbf{x})$ for t .

例 e.g. $y(\mathbf{x}, \mathbf{w}_{\text{ML}})$

損失関数 Loss function $L(t, f(\mathbf{x}))$

例 e.g. $L(t, f(\mathbf{x})) = \{f(\mathbf{x}) - t\}^2$

期待損失 Expected loss $\mathbb{E}[L] = \iint L(t, f(\mathbf{x}))p(\mathbf{x}, t) d\mathbf{x} dt$

決定理論 Decision theory

$\mathbb{E}[L]$ を最小にする $f(\mathbf{x})$ を選ぶ.

Choose $f(\mathbf{x})$ so as to minimize $\mathbb{E}[L]$.

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

変分法 Calculus of variations

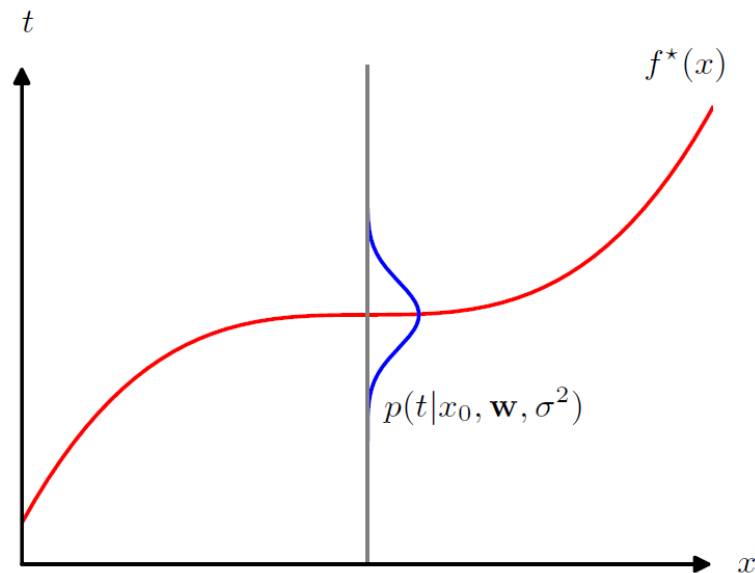
$$\frac{\delta \mathbb{E}[L]}{\delta f(\mathbf{x})} = 2 \int \{f(\mathbf{x}) - t\} p(\mathbf{x}, t) \, dt = 0$$

$$\rightarrow f^*(\mathbf{x}) = \frac{1}{p(\mathbf{x})} \int t p(\mathbf{x}, t) \, dt = \int t p(t|\mathbf{x}) \, dt = \mathbb{E}_t[t|\mathbf{x}]$$

$p(t|\mathbf{x}, \mathbf{w}, \sigma^2) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \sigma^2)$ に対しては,

For $p(t|\mathbf{x}, \mathbf{w}, \sigma^2) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \sigma^2)$,

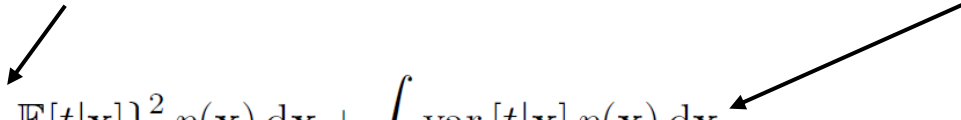
$$\mathbb{E}[t|\mathbf{x}] = \int t p(t|\mathbf{x}) \, dt = y(\mathbf{x}, \mathbf{w})$$



決定理論 Decision theory

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

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

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


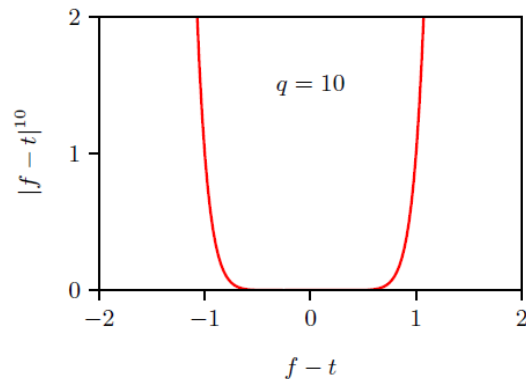
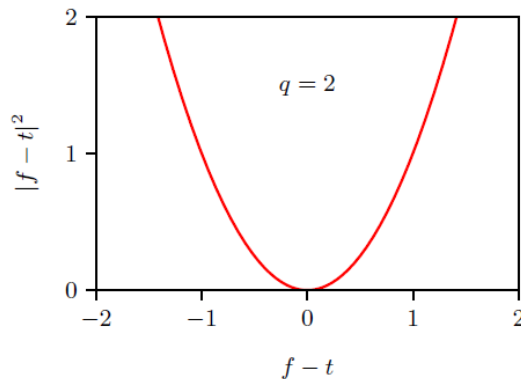
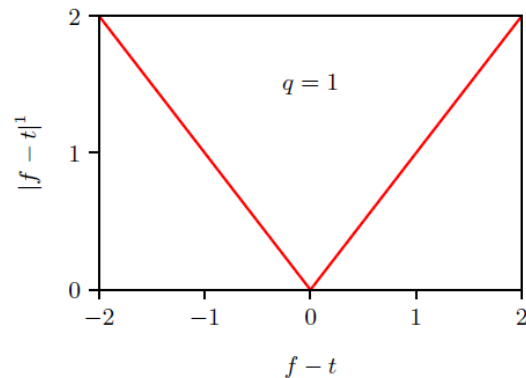
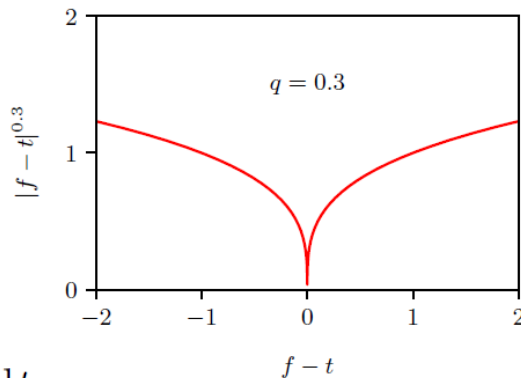
$\mathbb{E}[L]$ は $f(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}]$ のとき最小.

$\mathbb{E}[L]$ is minimized when $f(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}]$.

決定理論 Decision theory

ミンコフスキー損失
Minkowski loss

$$\mathbb{E}[L_q] = \iint |f(\mathbf{x}) - t|^q p(\mathbf{x}, t) d\mathbf{x} dt$$



バイアス-バリエアンスのトレードオフ The bias-variance trade-off

期待二乗損失関数は

Recall the expected squared loss function

$$\mathbb{E}[L] = \int \{f(\mathbf{x}) - h(\mathbf{x})\}^2 p(\mathbf{x}) d\mathbf{x} + \underbrace{\int \int \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) d\mathbf{x} dt}_{\text{noise}} \quad \uparrow$$

ただし
where

$$h(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}] = \int t p(t|\mathbf{x}) dt$$

$\mathbb{E}[L]$ の第二項は t に内在するノイズに相当.

The second term of $\mathbb{E}[L]$ corresponds to the noise inherent in t .

第一項は？

What about the first term?

バイアス-バリエアンスのトレードオフ The bias-variance trade-off

$\{f(\mathbf{x}; \mathcal{D}) - h(\mathbf{x})\}^2$ あるデータ集合 \mathcal{D} に対して
for a particular data set \mathcal{D}

$$\begin{aligned} \rightarrow & \{f(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})] + \mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}^2 \\ &= \{f(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})]\}^2 + \{\mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}^2 \\ &+ 2\{f(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})]\}\{\mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}. \end{aligned}$$

期待二乗損失関数の第一項

The first term of the expected squared loss function

$$\begin{aligned} & \mathbb{E}_{\mathcal{D}} [\{f(\mathbf{x}; \mathcal{D}) - h(\mathbf{x})\}^2] \\ &= \underbrace{\{\mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}} [\{f(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})]\}^2]}_{\text{variance}} \end{aligned}$$

バイアス-バリエーションのトレードオフ The bias-variance trade-off

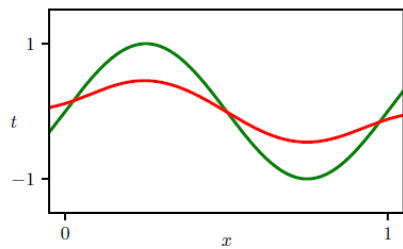
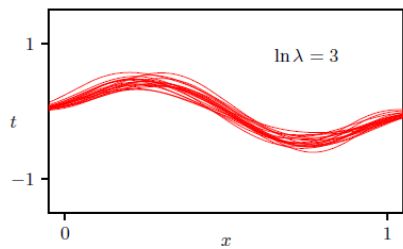
期待損失 = (バイアス)² + バリエーション + ノイズ
expected loss = (bias)² + variance + noise

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

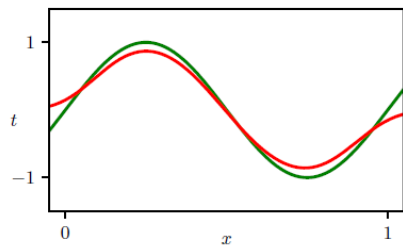
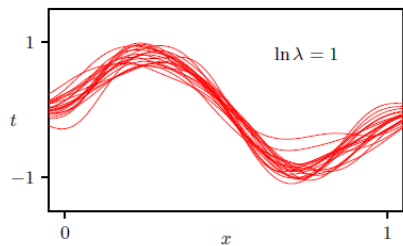
$$\text{variance} = \int \mathbb{E}_{\mathcal{D}} [\{f(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[f(\mathbf{x}; \mathcal{D})]\}^2] p(\mathbf{x}) d\mathbf{x}$$

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

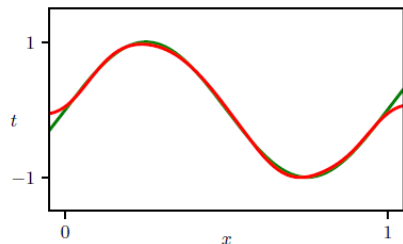
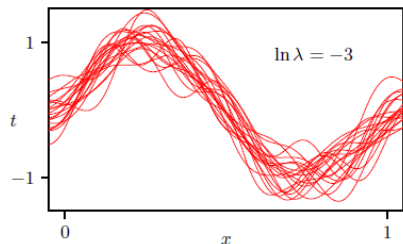
バイアス-バリエアンスのトレードオフ The bias-variance trade-off



バイアスが大きくバリエアンスが小さい
High bias and low variance



バイアスが小さくバリエアンスが大きい
Low bias and high variance

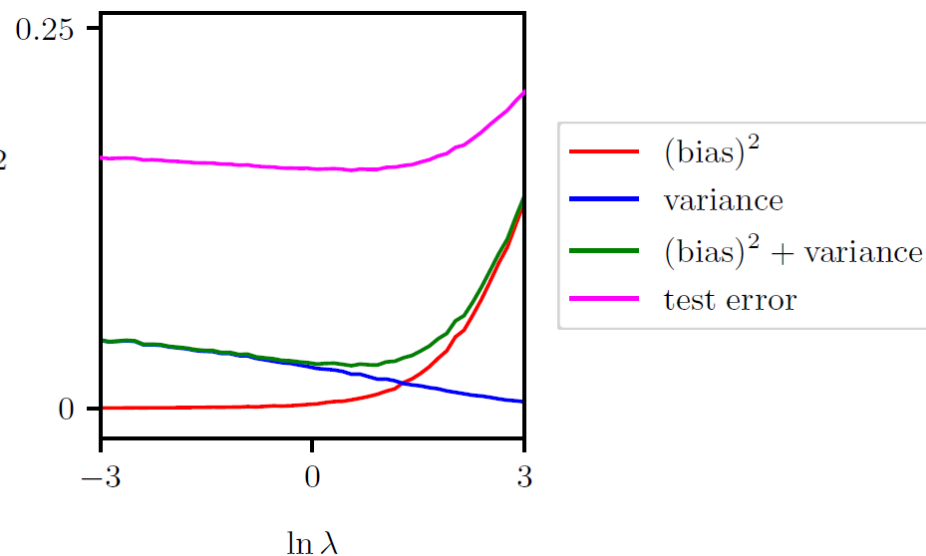


バイアス-バリアンスのトレードオフ The bias-variance trade-off

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

$$\text{variance} = \frac{1}{N} \sum_{n=1}^N \frac{1}{L} \sum_{l=1}^L \{f^{(l)}(x_n) - \bar{f}(x_n)\}^2$$

ただし
where $\bar{f}(x) = \frac{1}{L} \sum_{l=1}^L f^{(l)}(x)$





提出課題 II : 線形回帰モデル

Assignment II: Linear Models for Regression

提出期限 : **10月29日 (火曜日) 23:59:00** [日本標準時]

Submission deadline: **October 29 (Tuesday) 23:59:00** [Japan Standard Time]

提出課題は「一般」チャンネルの「ファイル」にアップロードされます。
同チャンネルに出現する通知のリンク先から解答を送信（提出）してください。
Assignments will be uploaded to "File" in the "General" channel. Send
(submit) your answers via the link that will appear in the same channel.

- 全6回の課題への解答をもとに成績評価を行います。
Your grades will be based on your answers to all six assignments.
- 解答送信後の解答再送信はできません。
Once submitted, answers cannot be resubmitted.
- 提出期限は一切延長しません。
The submission deadline will never be extended.