Linear models for regression

Lecture 2

Simplest model:

$$y(\vec{x}, \vec{w}) = w_0 + \sum_{j=1}^{D} w_j x_j$$

$\{\vec{x}_1 \dots \vec{x}_N\}$ multi-D observations $\rightarrow$ each $\vec{x} = \{x_1 \dots x_D\}$

$\{t_1 \dots t_N\}$ target variables

More generally,

$$y(\vec{x}, \vec{w}) = \underbrace{w_0}_{\text{bias prm}} + \sum_{j=1}^{D} w_j \underbrace{\varphi_j(\vec{x})}_{\text{basis f's}}$$

still a linear model because y is linear in $\vec{w}$

Sometimes, one defines $\varphi_0(\vec{x}) = 1$, s.t.

$$y(\vec{x}, \vec{w}) = \sum_{j=0}^{D} w_j \varphi_j(\vec{x}) = \vec{w}^T \cdot \vec{\varphi}(\vec{x})$$

$$\vec{w} = (w_0 \dots w_D) \qquad \vec{\varphi} = (\varphi_0 \dots \varphi_D)$$

Popular choices of basis f's: (1D examples)

(1) Gaussian $\varphi_j(x) = e^{-\frac{(x-\mu_j)^2}{2s^2}}$

(2) Sigmoidal $\varphi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$, where

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

As before, we assume that

$$\underset{\text{target}}{\underset{\uparrow}{t}} = \underset{\text{model}}{\underset{\uparrow}{y(\vec{x},\vec{w})}} + \underset{\text{noise}}{\underset{\uparrow}{\xi}}$$

$$p(\xi|\beta) = \mathcal{N}(0, \beta^{-1})$$

Correspondingly,

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

Now consider $\vec{X} = \{\underbrace{\vec{x}_1, \ldots, \vec{x}_N}_{\text{inputs}}\}$

$\vec{t} = \{\underbrace{t_1, \ldots, t_N}_{\text{target vars}}\}$

Under the independence assumption,

$$P(\vec{t}|\underset{\substack{\text{drop conditional dependence}\\ \text{on } \vec{X} \text{ for brevity}}}{\vec{X}},\vec{w},\beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|\vec{w}^T\cdot\vec{\varphi}(\vec{x}_n),\beta^{-1})$$

Then

$$(**)$$

$$\log P(\vec{t}|\vec{w},\beta) = \frac{N}{2}\log\beta - \frac{N}{2}\log(2\pi) - \beta\underbrace{\frac{1}{2}\sum_{n=1}^{N}(t_n-\vec{w}^T\vec{\varphi}(\vec{x}_n))^2}_{E_D(\vec{w})}$$

$$= \sum_{n=1}^{N}\log\mathcal{N}(t_n|\vec{w}^T\vec{\varphi}(x_n),\beta^{-1})$$

Now, use ML to determine $\vec{w}_{ML}$ & β_{ML}.
Start with the weights:

$$\frac{\partial}{\partial w_j} \log P(\vec{t}\,|\,\vec{w},\beta) = \frac{\beta}{\cancel{2}}\cancel{2}\sum_{n=1}^{N}\left(t_n - \vec{w}^T\vec{\varphi}(\vec{x}_n)\right)\times \varphi_j(\vec{x}_n),$$

or

$$\underbrace{\vec{\nabla}_{\vec{w}} \log P}_{=0} = \beta\sum_{n=1}^{N}\left(t_n - \vec{w}^T\vec{\varphi}(\vec{x}_n)\right)\vec{\varphi}(\vec{x}_n) = 0$$

$$\Rightarrow \sum_{n=1}^{N} t_n\,\varphi_j(\vec{x}_n) = \sum_{i=0}^{D} w_i \sum_{n=1}^{N}\varphi_i(\vec{x}_n)\,\varphi_j(\vec{x}_n)$$

Call $\varphi_j(\vec{x}_n) = \phi_{nj}$ → elements of $N\times(D+1)$ <u>design matrix</u>

Then
$$\underbrace{\overbrace{\sum_n t_n\phi_{nj}}^{(\phi^T\vec{t})_j}}_{\substack{D+1\\ \text{vector}}} = \sum_i w_i \underbrace{\sum_n \phi_{ni}\phi_{nj}}_{\substack{(D+1)\times(D+1)\\ \text{matrix}}} = \underbrace{\sum_i (\phi^T\phi)_{ji}\,w_i}_{\substack{D+1\\ \text{vector}}}$$

Finally,
$$\phi^T\vec{t} = (\phi^T\phi)\,\vec{w}\,, \quad \text{or}$$

$$\vec{w}_{ML} = (\phi^T\phi)^{-1}\phi^T\vec{t}$$

normal eq's for the least-squares problem

$$\phi = \begin{pmatrix} \varphi_0(\vec{x}_1) & \varphi_1(\vec{x}_1) & \dots & \varphi_D(\vec{x}_1) \\ \vdots & \vdots & & \vdots \\ \varphi_0(\vec{x}_N) & \varphi_1(\vec{x}_N) & \dots & \varphi_D(\vec{x}_N) \end{pmatrix}$$

$\tilde{\Phi} = (\Phi^T \Phi)^{-1} \Phi^T$ is called the Moore - Penrose pseudo-inverse of Φ.

Next, consider

$$E(\vec{w}) = \frac{1}{2} \sum_{n=1}^{N} \left(t_n - w_0 - \sum_{j=1}^{D} w_j \varphi_j(\vec{x}_n) \right)^2 .$$

$$\frac{\partial E}{\partial w_0} = - \sum_{n=1}^{N} \left(t_n - w_0 - \sum_{j=1}^{D} w_j \varphi_j(\vec{x}_n) \right) = 0$$

gives

$$w_0^{ML} = \frac{1}{N} \sum_{n=1}^{N} t_n - \frac{1}{N} \sum_{n=1}^{N} \sum_{j=1}^{D} w_j \varphi_j(\vec{x}_n) =$$

$$= \bar{t} - \sum_{j=1}^{D} w_j \bar{\varphi}_j \quad , \text{ where } \bar{\ldots} \text{ indicates } \frac{1}{N} \sum_{n=1}^{N} \ldots$$

Thus w_0^{ML} is the difference between the average of the target values and the weighted sum of basis f'n averages.

Finally, maximize (**) wrt β:

$$\frac{1}{\beta_{ML}} = \underbrace{\frac{1}{N} \sum_{n=1}^{N} \left(t_n - \vec{w}_{ML}^T \vec{\varphi}(\vec{x}_n) \right)^2}_{\text{residual variance of the target values around } y(\vec{x}, \vec{w})}$$

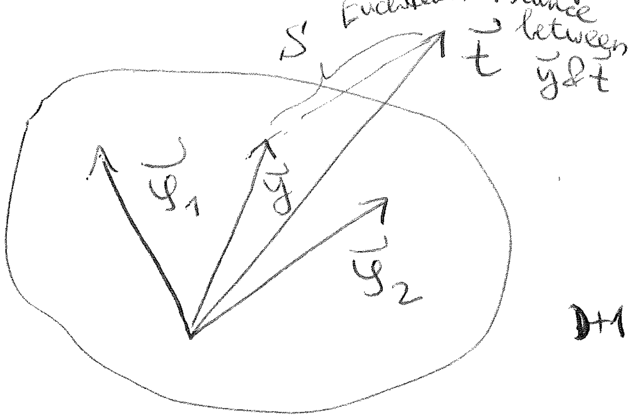
Geometry of least squares

$\vec{t} = (t_1 \dots t_N)$ is an N-dim vector

Each $\vec{\varphi}_j = (\varphi_j(\vec{x}_1) \dots \varphi_j(\vec{x}_N))$ is also an N-dim vector

[$\vec{\varphi}_j$ is the j^{th} column of Φ]

If $\underbrace{D+1}_{\text{the \# of basis functions, including } \varphi_0(\vec{x}_n)} < \overbrace{N}^{\text{\# datapoints}}$, then $\vec{\varphi}_j$ vectors will span a subspace S' of dimensionality $D+1$ in the N-dim'l space.



Define $\vec{y} = (y(\vec{x}_1, \vec{w}) \dots y(\vec{x}_N, \vec{w}))$ N-dim vector, a linear combination of $D+1$ $\vec{\varphi}_j$ vectors.

$E(\vec{w}) \sim$ ~~second~~ square of Euclidean dist. between $\vec{y}$ & $\vec{t}$, so we need to minimize it. This is accomplished by the orthogonal projection of $\vec{t}$ into subspace S'.

In practice, $\Phi^T\Phi$ may be hard to invert, when some $\vec{\varphi}_j$'s are nearly colinear $\rightarrow$ add a regularization term to prevent this.

Regularized least squares

Consider now

$$\widetilde{E}(\vec{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(t_n - \vec{w}^T \vec{\varphi}(\vec{x}_n)\right)^2 + \frac{\lambda}{2}\vec{w}^T\vec{w}$$

still a quadratic f'n of w_j

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

$\vec{w}^* = (\lambda \mathbb{I} + \Phi^T\Phi)^{-1}\Phi^T\vec{t}$. [the inverse matrix is now regularized]

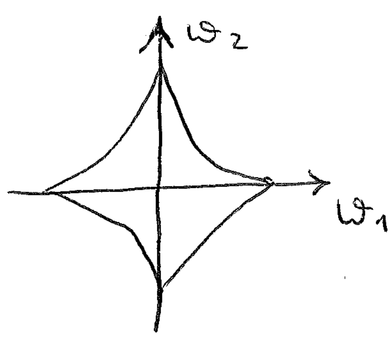
$\mathbb{I}$ unit matrix $(D+1)\times(D+1)$

More generally,

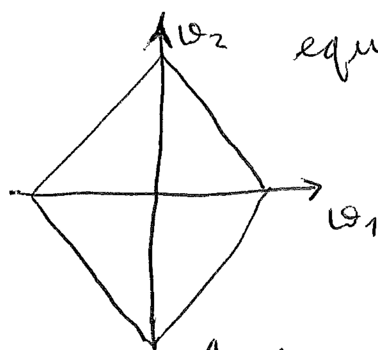
$$\widetilde{E}(\vec{w}) = \frac{1}{2}\sum_{n=1}^{N}(\ldots)^2 + \frac{\lambda}{2}\sum_{j=1}^{D+1}|w_j|^q$$

$q = 2 \leftarrow$ quadratic regularizer above

$q = 1 \leftarrow$ LASSO regularizer

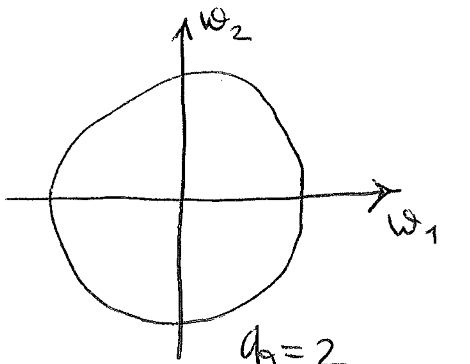


$q=0.5$

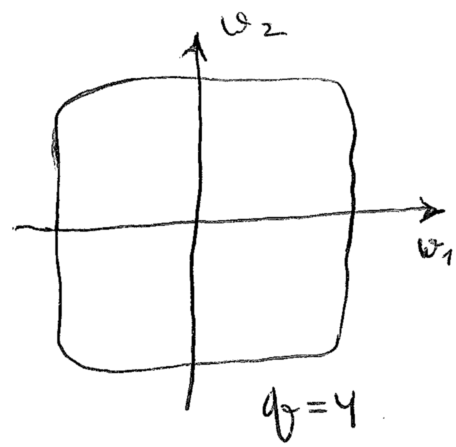


$q=1$

equal value contours

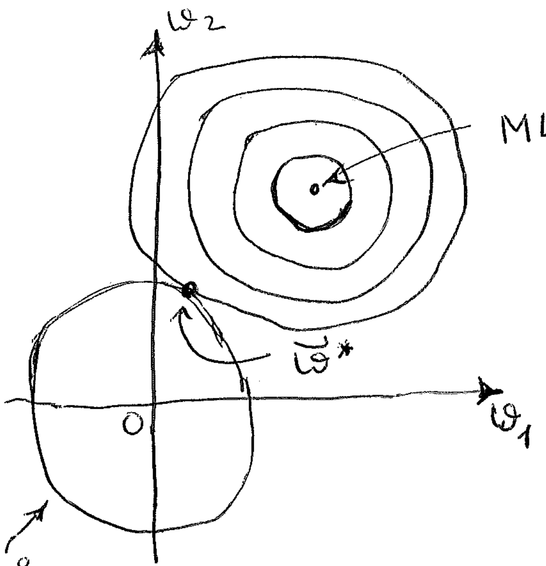


$q=2$



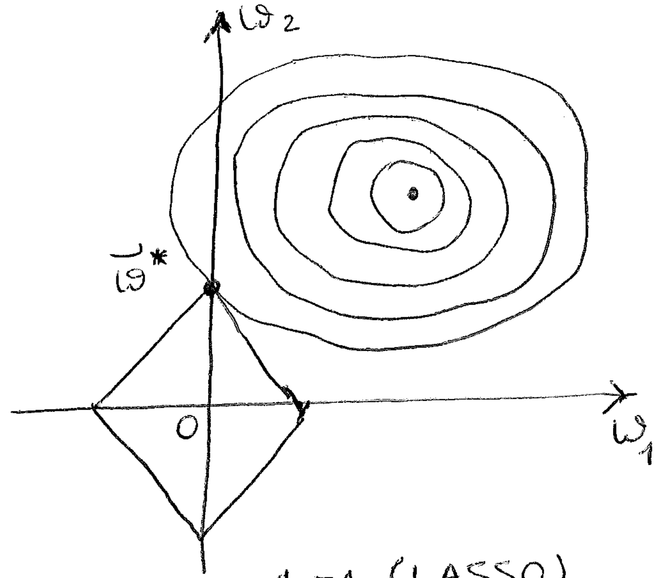
$q=4$

Now, consider



sphere centered on Ø

$q = 2$



$q = 1$ (LASSO) results in (sparse solution)

Loss functions for regression (1.5.5)

Consider $\underset{\text{input}}{\vec{x}} \to \underset{\text{target}}{t}$

$$\underset{\substack{\text{model}\\ \text{for } t}}{y(\vec{x})} \to \underset{\text{loss}}{L(t, y(\vec{x}))} \overset{\text{e.g.}}{=} \underbrace{(y(\vec{x}) - t)^2}_{\text{squared loss}}$$

$$\underset{\substack{\text{expected}\\ \text{value of}\\ \text{loss}}}{E[L]} = \int d\vec{x}\, dt\, \underbrace{p(\vec{x}, t)}_{\substack{\text{joint prob.}\\ \text{of } \vec{x} \,\&\, t}} \underbrace{(y(\vec{x}) - t)^2}_{\text{loss f'n}}$$

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

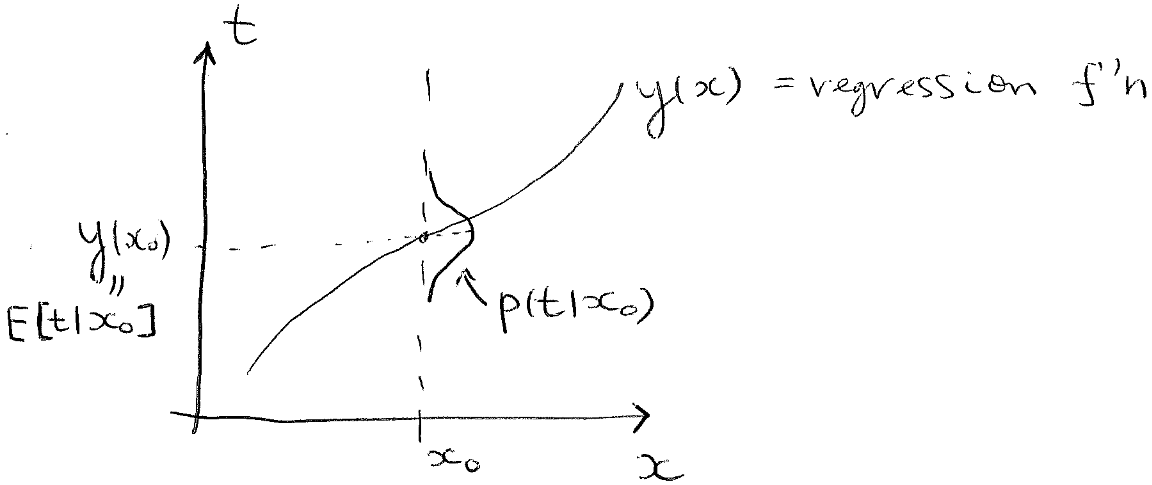
minimize E[L]

$\Downarrow$

$$y(\vec{x}) = \frac{\int dt\, p(\vec{x}, t)\, t}{p(\vec{x})} = \int dt\, t\, p(t|\vec{x}) =$$

$$= E[t|\vec{x}] \qquad (+)$$

$y(\vec{x})$ is called a <u>regression</u> <u>f'n</u>



Further,

$$(y(\vec{x})-t)^2 = (y(\vec{x})-E[t|\vec{x}]+E[t|\vec{x}]-t)^2 =$$

$$= (y(\vec{x})-E)^2 + 2(y(\vec{x})-E)(E-t) + (E-t)^2$$

Then $$E[L] = \int dt\,d\vec{x}\; p(\vec{x},t)\left[(y(\vec{x}) - \overbrace{E[t|\vec{x}]}^{\text{f'n of } \vec{x}\text{, not } t})^2 + \right.$$

$$\left. + 2(y(\vec{x})-E[t|\vec{x}])(E[t|\vec{x}]-t) + (E[t|\vec{x}]-t)^2\right] =$$

$$= \int d\vec{x}\, p(\vec{x})\, (y(\vec{x})-E[t|\vec{x}])^2 +$$

$$+ 2\int d\vec{x}\,(y(\vec{x})-E[t|\vec{x}])\underbrace{\int dt\, \overbrace{p(\vec{x},t)}^{p(t|\vec{x})p(\vec{x})}(E[t|\vec{x}]-t)}_{E[t|\vec{x}]\,p(\vec{x}) \;-\; p(\vec{x})\,E[t|\vec{x}] \;=0} +$$

2nd term vanishes

$$+ \int dt\,d\vec{x}\; p(\vec{x},t)\,(E[t|\vec{x}]-t)^2 .$$

Only the 1<u>st</u> term depends on $y(\vec{x})$, and will be $=0$ (at min) iff

$y(\vec{x}) = E[t|\vec{x}]$, consistent with (+)

The 3rd term represents noise in the target values & is indep. of the model:

$$\int d\vec{x}\, \underbrace{p(\vec{x})\, E^2[t|x]} - 2\int dt\, d\vec{x}\; t\, p(\vec{x},t)\, E[t,\vec{x}] +$$

$$+ \int dt\, t^2 p(t) =$$

$$= \int d\vec{x}\; \frac{\int dt\, t\, p(\vec{x},t) \int dt'\, t'\, p(\vec{x},t')}{p(\vec{x})} -$$

$p(t|\vec{x}) = \frac{p(\vec{x},t)}{p(\vec{x})} \rightarrow$

$$-2\int dt\, d\vec{x}\; t\, p(\vec{x},t)\, \frac{\int dt'\, t'\, p(\vec{x},t')}{p(\vec{x})} + \overbrace{\int dt\, t^2 p(t)}^{\langle t^2\rangle} =$$

$$= \langle t^2 \rangle - \underbrace{\int \frac{d\vec{x}}{p(\vec{x})} \int dt\, t\, p(\vec{x},t) \int dt'\, t'\, p(\vec{x},t')}.$$

$$\int d\vec{x}\, p(\vec{x}) \left(\underbrace{\frac{\int dt\, t\, p(\vec{x},t)}{\int dt\, p(\vec{x},t)}}_{= \langle t \rangle_{(\vec{x})} \;\left(\text{f'n of } \vec{x}\right)} \right)^2 = \int d\vec{x}\, p(\vec{x}) \langle t(\vec{x}) \rangle^2$$

$$\langle t^2 \rangle = \int dt\, t^2 p(t) = \frac{\int dt\, d\vec{x}\; t^2 p(\vec{x},t)}{\underbrace{\int dt\, d\vec{x}\, p(\vec{x},t)}_{=1}} = \int d\vec{x}\, \langle t^2(\vec{x}) \rangle\, p(\vec{x})$$

$\langle .. \rangle$ signifies an average wrt $p(\vec{x},t)$

$$\langle t^2(\vec{x}) \rangle = \frac{\int dt\, t^2 p(\vec{x},t)}{\underbrace{\int dt\, p(\vec{x},t)}_{p(\vec{x})}}.$$

So, $\int dt\, d\vec{x}\, p(\vec{x},t) \left(E[t|\vec{x}] - t \right)^2 =$
$= \int d\vec{x}\, p(\vec{x}) \left[\langle t^2(\vec{x}) \rangle - \langle t(\vec{x}) \rangle^2 \right].$