Error-based Learning
Sections 7.4, 7.5

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Interpreting Multivariable Linear Regression Models

- The weights used by linear regression models indicate the effect of each descriptive feature on the predictions returned by the model.
- Both the **sign** and the **magnitude** of the weight provide information on how the descriptive feature effects the predictions of the model.

Table: Weights and standard errors for each feature in the office rentals model.

Descriptive Feature	Weight	Standard Error	*t*-statistic	*p*-value
SIZE	0.6270	0.0545	11.504	$<$0.0001
FLOOR	-0.1781	2.7042	-0.066	0.949
BROADBAND RATE	0.071396	0.2969	0.240	0.816

- It is tempting to infer the relative importance of the different descriptive features in the model from the magnitude of the weights
- However, direct comparison of the weights tells us little about their relative importance.
- A better way to determine the importance of each descriptive feature in the model is to perform a **statistical significance test**.

- The statistical significance test we use to analyze the importance of a descriptive feature $\mathbf{d}[j]$ in a linear regression model is the ***t*-test**.
- The null hypothesis for this test is that the feature does not have a significant impact on the model. The test statistic we calculate is called the *t*-statistic.

- The standard error for the overall model is calculated as

$$se = \sqrt{\frac{\sum_{i=1}^{n} (t_i - \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i))^2}{n-2}} \tag{1}$$

- A standard error calculation is then done for a descriptive feature as follows:

$$se(\mathbf{d}[j]) = \frac{se}{\sqrt{\sum_{i=1}^{n} \left(\mathbf{d}_i[j] - \overline{\mathbf{d}[j]}\right)^2}} \tag{2}$$

- The *t*-statistic for this test is calculated as follows:

$$t = \frac{\mathbf{w}[j]}{se(\mathbf{d}[j])} \tag{3}$$

- Using a standard *t*-statistic look-up table, we can then determine the *p*-value associated with this test (this is a two tailed *t*-test with degrees of freedom set to the number of instances in the training set minus 2).
- If the *p*-value is less than the required significance level, typically 0.05, we reject the null hypothesis and say that the descriptive feature has a significant impact on the model; otherwise we say that it does not.

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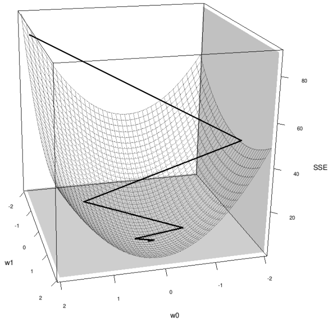
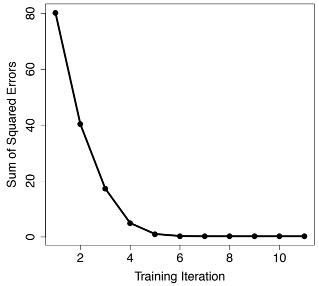
Setting the Learning Rate Using Weight Decay

- **Learning rate decay** allows the learning rate to start at a large value and then decay over time according to a predefined schedule.
- A good approach is to use the following decay schedule:

$$\alpha_\tau = \alpha_0 \frac{c}{c+\tau} \tag{4}$$

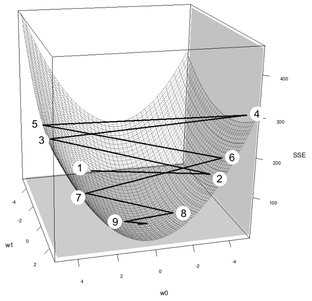


(a)

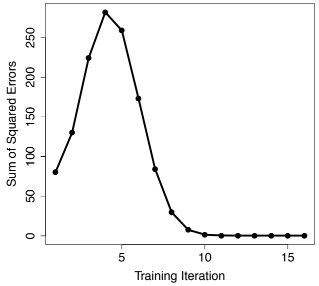


(b)

Figure: (a) The journey across the error surface for the office rentals prediction problem when learning rate decay is used ($\alpha_0 = 0.18$, $c = 10$); (b) a plot of the changing sum of squared error values during this journey.



(a)



(b)

Figure: (a) The journey across the error surface for the office rentals prediction problem when learning rate decay is used ($\alpha_0 = 0.25$, $c = 100$); (b) a plot of the changing sum of squared error values during this journey.

Handling Categorical Descriptive Features

- The basic structure of the multivariable linear regression model allows for only continuous descriptive features, so we need a way to handle categorical descriptive features.
- The most common approach to handling categorical features uses a transformation that converts a single categorical descriptive feature into a number of continuous descriptive feature values that can encode the levels of the categorical feature.
- For example, the ENERGY RATING descriptive feature would be converted into three new continuous descriptive features, as it has 3 distinct levels: *'A'*, *'B'*, or *'C'*.

Table: The office rentals dataset adjusted to handle the categorical ENERGY RATING descriptive feature in linear regression models.

ID	SIZE	FLOOR	BROADBAND RATE	ENERGY RATING A	ENERGY RATING B	ENERGY RATING C	RENTAL PRICE
1	500	4	8	0	0	1	320
2	550	7	50	1	0	0	380
3	620	9	7	1	0	0	400
4	630	5	24	0	1	0	390
5	665	8	100	0	0	1	385
6	700	4	8	0	1	0	410
7	770	10	7	0	1	0	480
8	880	12	50	1	0	0	600
9	920	14	8	0	0	1	570
10	1 000	9	24	0	1	0	620

- Returning to our example, the regression equation for this RENTAL PRICE model would change to

$$\begin{aligned}\text{RENTAL PRICE} = \mathbf{w}[0] &+ \mathbf{w}[1] \times \text{SIZE} + \mathbf{w}[2] \times \text{FLOOR}\\ &+ \mathbf{w}[3] \times \text{BROADBAND RATE}\\ &+ \mathbf{w}[4] \times \text{ENERGY RATING A}\\ &+ \mathbf{w}[5] \times \text{ENERGY RATING B}\\ &+ \mathbf{w}[6] \times \text{ENERGY RATING C}\end{aligned}$$

  where the newly added categorical features allow the original ENERGY RATING feature to be included.

Handling Categorical Target Features: Logistic Regression

Table: A dataset listing features for a number of generators.

ID	RPM	VIBRATION	STATUS
1	568	585	good
2	586	565	good
3	609	536	good
4	616	492	good
5	632	465	good
6	652	528	good
7	655	496	good
8	660	471	good
9	688	408	good
10	696	399	good
11	708	387	good
12	701	434	good
13	715	506	good
14	732	485	good
15	731	395	good
16	749	398	good
17	759	512	good
18	773	431	good
19	782	456	good
20	797	476	good
21	794	421	good
22	824	452	good
23	835	441	good
24	862	372	good
25	879	340	good
26	892	370	good
27	913	373	good
28	933	330	good
29	562	309	faulty
30	578	346	faulty
31	593	357	faulty
32	626	341	faulty
33	635	252	faulty
34	658	235	faulty
35	663	299	faulty
36	677	223	faulty
37	685	303	faulty
38	698	197	faulty
39	699	311	faulty
40	712	257	faulty
41	722	193	faulty
42	735	259	faulty
43	738	314	faulty
44	753	113	faulty
45	767	286	faulty
46	771	264	faulty
47	780	137	faulty
48	784	131	faulty
49	798	132	faulty
50	820	152	faulty
51	834	157	faulty
52	858	163	faulty
53	888	91	faulty
54	891	156	faulty
55	911	79	faulty
56	939	99	faulty

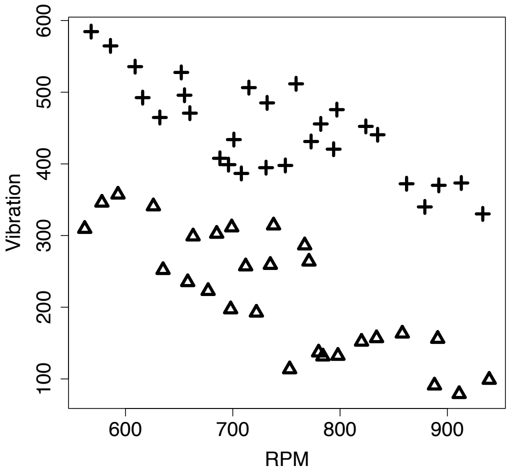


Figure: A scatter plot of the RPM and VIBRATION descriptive features from the generators dataset shown in Table 4 [18] where *'good'* generators are shown as crosses and *'faulty'* generators are shown as triangles.

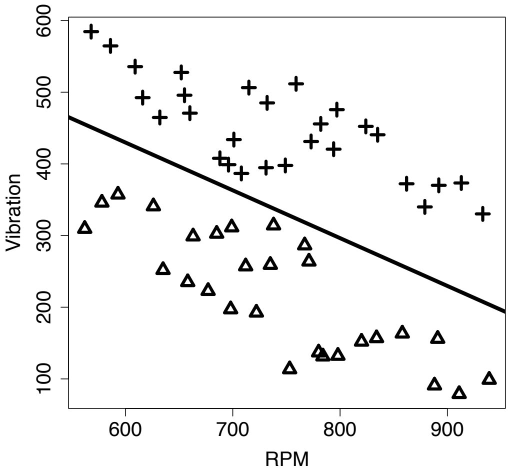


Figure: A scatter plot of the RPM and VIBRATION descriptive features from the generators dataset shown in Table 4 [18]. A decision boundary separating *'good'* generators (crosses) from *'faulty'* generators (triangles) is also shown.

- As the decision boundary is a **linear separator** it can be defined using the equation of the line as:

$$\textsc{Vibration} = 830 - 0.667 \times \textsc{RPM} \tag{5}$$

or

$$830 - 0.667 \times \textsc{RPM} - \textsc{Vibration} = 0 \tag{6}$$

- Applying Equation (6)[21] to the instance RPM $= 810$, VIBRATION $= 495$, which is be above the decision boundary, gives the following result:

$$830 - 0.667 \times 810 - 495 = -205.27$$

- By contrast, if we apply Equation (6)[21] to the instance RPM $= 650$ and VIBRATION $= 240$, which is be below the decision boundary, we get

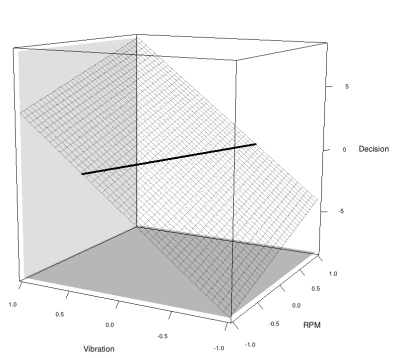
$$830 - 0.667 \times 650 - 240 = 156.45$$

- All the data points above the decision boundary will result in a negative value when plugged into the decision boundary equation, while all data points below the decision boundary will result in a positive value.

- Reverting to our previous notation we have:

$$\mathbb{M}_{\mathbf{w}}(\mathbf{d}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \mathbf{d} \geq 0 \\ 0 & \textit{otherwise} \end{cases} \tag{7}$$

- The surface defined by this rule is known as a **decision surface**.



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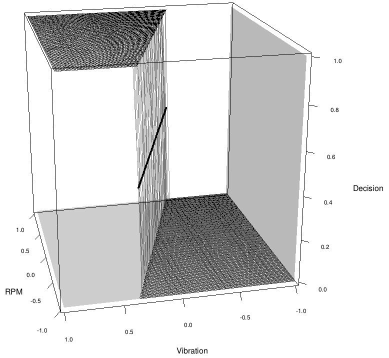


(b)

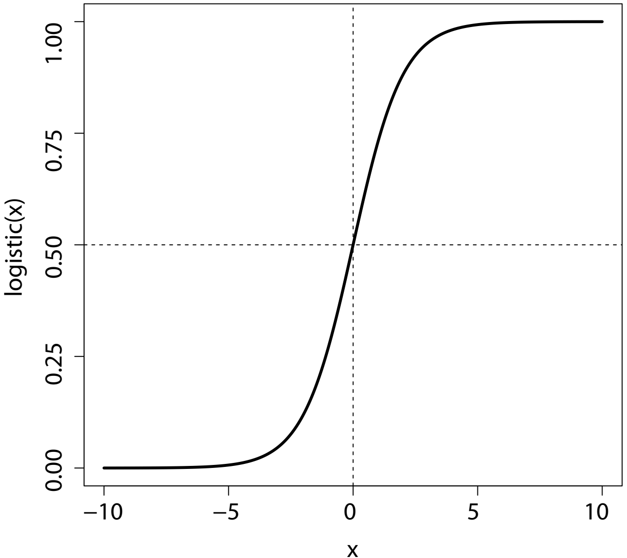
Figure: (a) A surface showing the value of Equation (6)[21] for all values of RPM and VIBRATION. The decision boundary given in Equation (6)[21] is highlighted. (b) The same surface linearly thresholded at zero to operate as a predictor.

- The hard decision boundary given in Equation (7)[24] is **discontinuous** so is not differentiable and so we can’t calculate the gradient of the error surface.
- Furthermore, the model always makes completely confident predictions of 0 or 1, whereas a little more subtlety is desirable.
- We address these issues by using a more sophisticated threshold function that is continuous, and therefore differentiable, and that allows for the subtlety desired: the **logistic function**

logistic function

$$Logistic(x) = \frac{1}{1 + e^{-x}} \tag{8}$$

where x is a numeric value and e is **Euler's number** and is approximately equal to 2.7183.


logistic(x)
x
0.00
0.25
0.50
0.75
1.00
−10
−5
0
5
10

- To build a logistic regression model, we simply pass the output of the basic linear regression model through the logistic function

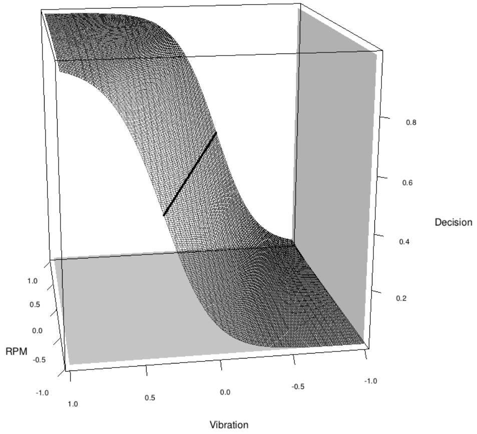
$$\begin{aligned}\mathbb{M}_{\mathbf{w}}(\mathbf{d}) &= Logistic(\mathbf{w} \cdot \mathbf{d}) \\ &= \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{d}}}\end{aligned} \tag{9}$$

A note on training logistic regression models:

1. Before we train a logistic regression model we map the binary target feature levels to 0 or 1.
2. The error of the model on each instance is then the difference between the target feature (0 or 1) and the value of the prediction $[0, 1]$.

Example

$$\mathbb{M}_{\mathbf{w}}(\langle \text{RPM}, \text{VIBRATION} \rangle) = \frac{1}{1 + e^{-(-0.4077 + 4.1697 \times \text{RPM} + 6.0460 \times \text{VIBRATION})}}$$



- The decision surface for the example logistic regression model.

$$P(t = \textit{'faulty'}|\mathbf{d}) = \mathbb{M}_{\mathbf{w}}(\mathbf{d})$$
$$P(t = \textit{'good'}|\mathbf{d}) = 1 - \mathbb{M}_{\mathbf{w}}(\mathbf{d})$$

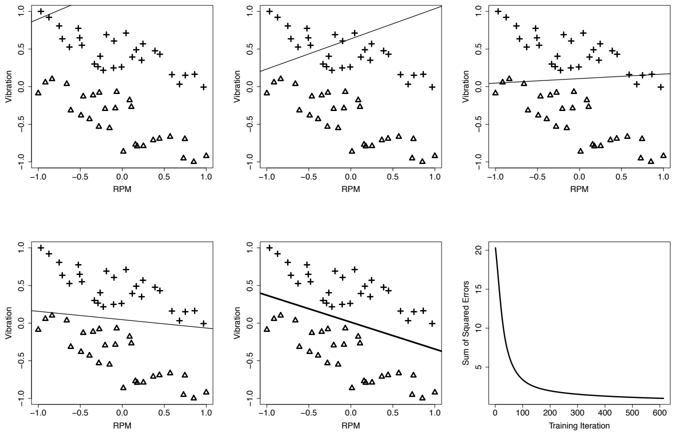


Figure: A selection of the logistic regression models developed during the gradient descent process for the machinery dataset from Table 4 [18]. The bottom-right panel shows the sum of squared error values generated during the gradient descent process.

- To repurpose the gradient descent algorithm for training logistic regression models the only change that needs to be made is i in the weight update rule.
- See pg. 360 in book for details of how to derive the new weight update rule.
- The new weight update rule is:

$$\mathbf{w}[j] \leftarrow \mathbf{w}[j] + \alpha \times \sum_{i=1}^{n} \left((t - \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i)) \times \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i) \times (1 - \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i)) \times \mathbf{d}_i[j] \right)$$

ID	RPM	VIBRATION	STATUS
1	498	604	faulty
2	517	594	faulty
3	541	574	faulty
4	555	587	faulty
5	572	537	faulty
6	600	553	faulty
7	621	482	faulty
8	632	539	faulty
9	656	476	faulty
10	653	554	faulty
11	679	516	faulty
12	688	524	faulty
13	684	450	faulty
14	699	512	faulty
15	703	505	faulty
16	717	377	faulty
17	740	377	faulty
18	749	501	faulty
19	756	492	faulty
20	752	381	faulty
21	762	508	faulty
22	781	474	faulty
23	781	480	faulty
24	804	460	faulty
25	828	346	faulty
26	830	366	faulty
27	864	344	faulty
28	882	403	faulty
29	891	338	faulty
30	921	362	faulty
31	941	301	faulty
32	965	336	faulty
33	976	297	faulty
34	994	287	faulty
35	501	463	good
36	526	443	good
37	536	412	good
38	564	394	good
39	584	398	good
40	602	398	good
41	610	428	good
42	638	389	good
43	652	394	good
44	659	336	good
45	662	364	good
46	672	308	good
47	691	248	good
48	694	401	good
49	718	313	good
50	720	410	good
51	723	389	good
52	744	227	good
53	741	397	good
54	770	200	good
55	764	370	good
56	790	248	good
57	786	344	good
58	792	290	good
59	818	268	good
60	845	232	good
61	867	195	good
62	878	168	good
63	895	218	good
64	916	221	good
65	950	156	good
66	956	174	good
67	973	134	good
68	1002	121	good

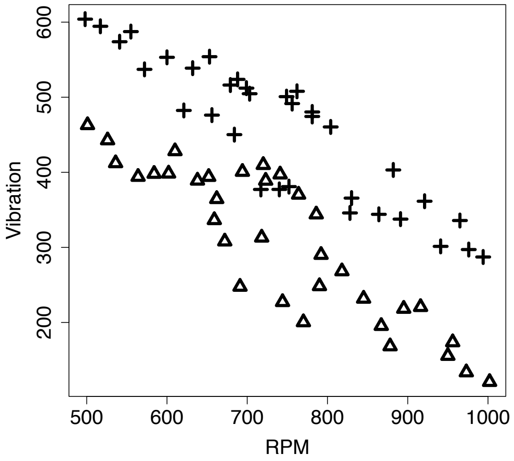


Figure: A scatter plot of the extended generators dataset given in Table 35 [35], which results in instances with the different target levels overlapping with each other. *'good'* generators are shown as crosses, and *'faulty'* generators are shown as triangles.

- For logistic regression models we recommend that descriptive feature values always be normalized.
- In this example, before the training process begins, both descriptive features are normalized to the range $[-1, 1]$.

- For this example let's assume that:
  - $\alpha = 0.02$

Initial Weights

w[0]:	-2.9465	**w**[1]:	-1.0147	**w**[2]:	-2.1610

Iteration 1

ID	TARGET LEVEL	Pred.	Error	Squared Error	errorDelta($\mathcal{D}$, **w**[**i**]) **w**[0]	**w**[1]	**w**[2]
1	1	0.5570	0.4430	0.1963	0.1093	-0.1093	0.1093
2	1	0.5168	0.4832	0.2335	0.1207	-0.1116	0.1159
3	1	0.4469	0.5531	0.3059	0.1367	-0.1134	0.1197
4	1	0.4629	0.5371	0.2885	0.1335	-0.1033	0.1244
				...			
65	0	0.0037	-0.0037	0.0000	0.0000	0.0000	0.0000
66	0	0.0042	-0.0042	0.0000	0.0000	0.0000	0.0000
67	0	0.0028	-0.0028	0.0000	0.0000	0.0000	0.0000
68	0	0.0022	-0.0022	0.0000	0.0000	0.0000	0.0000
			Sum	24.4738	2.7031	-0.7015	1.6493
Sum of squared errors (Sum/2)				12.2369			

$$\mathbf{w}[j] \leftarrow \mathbf{w}[j] + \alpha \times \sum_{i=1}^{n} \left((t_i - \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i)) \times \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i) \times (1 - \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i)) \times \mathbf{d}_i[j] \right)$$

New Weights (after Iteration 1)

w[0]:	-2.8924	**w**[1]:	-1.0287	**w**[2]:	-2.1940

Iteration 2

ID	TARGET LEVEL	Pred.	Error	Squared Error	errorDelta($\mathcal{D}$, **w**[**i**]) **w**[0]	**w**[1]	**w**[2]
1	1	0.5817	0.4183	0.1749	0.1018	-0.1018	0.1018
2	1	0.5414	0.4586	0.2103	0.1139	-0.1053	0.1094
3	1	0.4704	0.5296	0.2805	0.1319	-0.1094	0.1155
4	1	0.4867	0.5133	0.2635	0.1282	-0.0992	0.1194
...							
65	0	0.0037	-0.0037	0.0000	0.0000	0.0000	0.0000
66	0	0.0043	-0.0043	0.0000	0.0000	0.0000	0.0000
67	0	0.0028	-0.0028	0.0000	0.0000	0.0000	0.0000
68	0	0.0022	-0.0022	0.0000	0.0000	0.0000	0.0000
			Sum	24.0524	2.7236	-0.6646	1.6484
			Sum of squared errors (Sum/2)	12.0262			

$$\mathbf{w}[j] \leftarrow \mathbf{w}[j] + \alpha \times \sum_{i=1}^{n} \left(\left(t_i - \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i) \right) \times \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i) \times \left(1 - \mathbb{M}_{\mathbf{w}}(\mathbf{d}_i) \right) \times \mathbf{d}_i[j] \right)$$

New Weights (after Iteration 2)

w[0]:	-2.8380	**w**[1]:	-1.0416	**w**[2]:	-2.2271

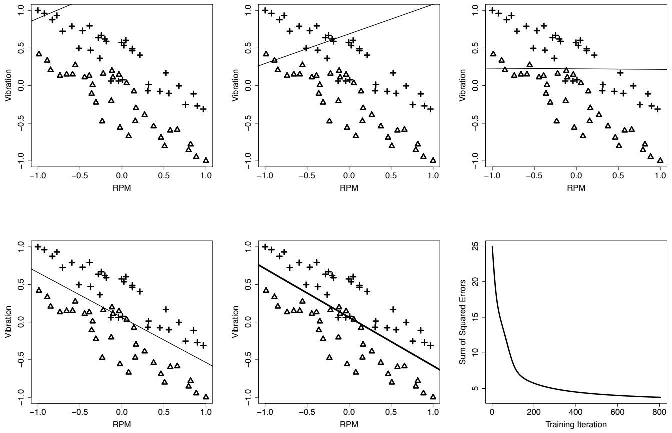


Figure: A selection of the logistic regression models developed during the gradient descent process for the extended generators dataset in Table 35 [35]. The bottom-right panel shows the sum of squared error values generated during the gradient descent process.

- The final model found is:

$$\mathbb{M}_{\mathbf{w}}(\langle \text{RPM}, \textsc{Vibration} \rangle) = \frac{1}{1 + e^{-(-0.4077 + 4.1697 \times \text{RPM} + 6.0460 \times \textsc{Vibration})}}$$

Modeling Non-linear Relationships

Table: A dataset describing grass growth on Irish farms during July 2012.

ID	RAIN	GROWTH
1	2.153	14.016
2	3.933	10.834
3	1.699	13.026
4	1.164	11.019
5	4.793	4.162
6	2.690	14.167
7	3.982	10.190
8	3.333	13.525
9	1.942	13.899
10	2.876	13.949
11	4.277	8.643
12	3.754	11.420
13	2.809	13.847
14	1.809	13.757
15	4.114	9.101
16	2.834	13.923
17	3.872	10.795
18	2.174	14.307
19	4.353	8.059
20	3.684	12.041
21	2.140	14.641
22	2.783	14.138
23	3.960	10.307
24	3.592	12.069
25	3.451	12.335
26	1.197	10.806
27	0.723	7.822
28	1.958	14.010
29	2.366	14.088
30	1.530	12.701
31	0.847	9.012
32	3.843	10.885
33	0.976	9.876

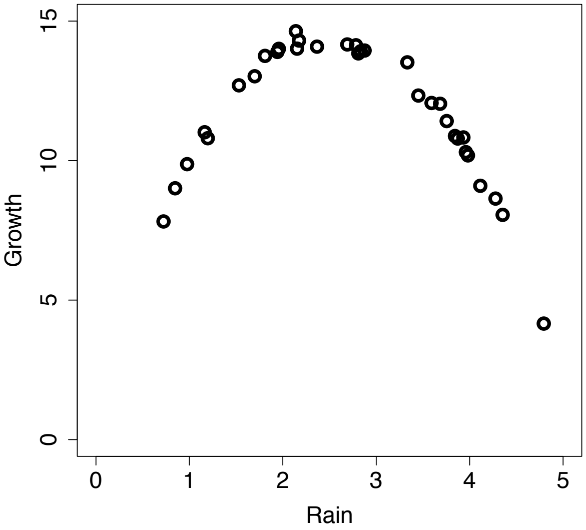


Figure: A scatter plot of the RAIN and GROWTH feature from the grass growth dataset.

- The best linear model we can learn for this data is:

$$\text{GROWTH} = 13.510 + -0.667 \times \text{RAIN}$$

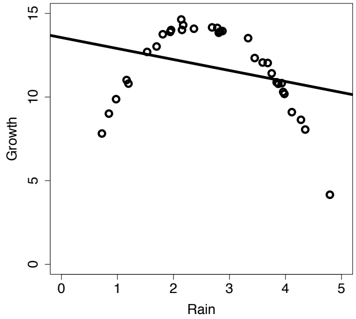


Figure: A simple linear regression model trained to capture the relationship between the grass growth and rainfall.

- In order to handle non-linear relationships we transform the data rather than the model using a set of basis functions:

$$\mathbb{M}_{\mathbf{w}}(\mathbf{d}) = \sum_{k=0}^{b} \mathbf{w}[k] \times \phi_k(\mathbf{d}) \tag{10}$$

where ϕ_0 to ϕ_b are a series of b basis functions that each transform the input vector **d** in a different way.
- The advantage of this is that, except for introducing the mechanism of basis functions, we do not need to make any other changes to the approach we have presented so far.

- The relationship between rainfall and grass growth in the grass growth dataset can be accurately represented as a **second order polynomial** through the following model:

$$\textsc{Growth} = \mathbf{w}[0] \times \phi_0(\textsc{Rain}) + \mathbf{w}[1] \times \phi_1(\textsc{Rain}) + \mathbf{w}[2] \times \phi_2(\textsc{Rain})$$

where

$$\begin{aligned} \phi_0(\textsc{Rain}) &= 1 \\ \phi_1(\textsc{Rain}) &= \textsc{Rain} \\ \phi_2(\textsc{Rain}) &= \textsc{Rain}^2 \end{aligned}$$

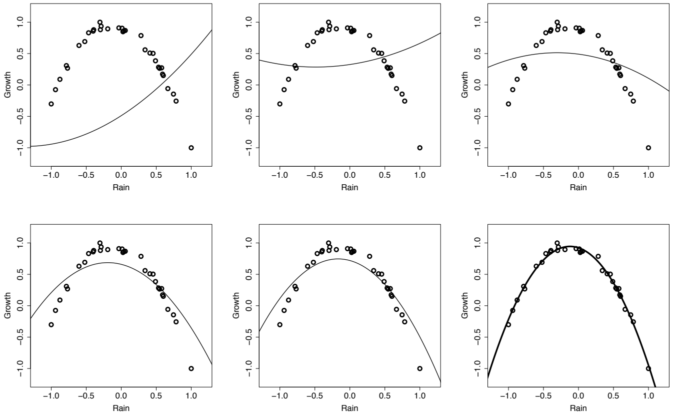
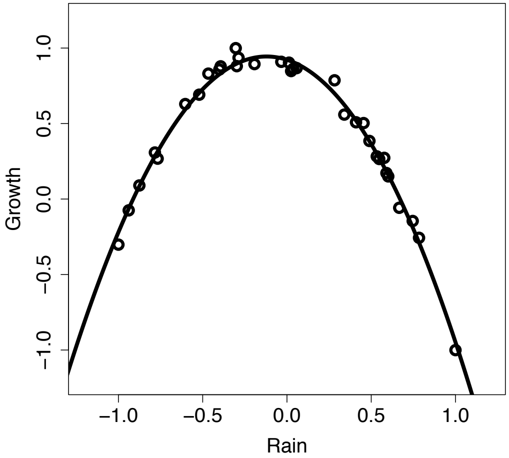


Figure: A selection of the models developed during the gradient descent process for the grass growth dataset from Table 5 [46]. (Note that the RAIN and GROWTH features have been **range normalized** to the $[-1, 1]$ range.)



$$\textsc{Growth} = 0.3707 \times \phi_0(\textsc{Rain}) + 0.8475 \times \phi_1(\textsc{Rain}) + -1.717 \times \phi_2(\textsc{Rain})$$

$$\textsc{Growth} = 0.3707 \times \phi_0(\textsc{Rain}) + 0.8475 \times \phi_1(\textsc{Rain}) + -1.717 \times \phi_2(\textsc{Rain})$$

$$\begin{aligned} \phi_0(\textsc{Rain}) &= 1 \\ \phi_1(\textsc{Rain}) &= \textsc{Rain} \\ \phi_2(\textsc{Rain}) &= \textsc{Rain}^2 \end{aligned}$$

- What is the predicted growth for the following RAIN values:
  1. RAIN$= -0.75$
  2. RAIN$= 0.1$
  3. RAIN$= 0.9$

- Basis functions can also be used for
  1. multivariable simple linear regression models in the same way, the only extra requirement being the definition of more basis functions.
  2. to train logistic regression models for categorical prediction problems that involve non-linear relationships.

Table: A dataset showing participants' responses to viewing *'positive'* and *'negative'* images measured on the EEG P20 and P45 potentials.

ID	P20	P45	TYPE	ID	P20	P45	TYPE
1	0.4497	0.4499	negative	26	0.0656	0.2244	positive
2	0.8964	0.9006	negative	27	0.6336	0.2312	positive
3	0.6952	0.3760	negative	28	0.4453	0.4052	positive
4	0.1769	0.7050	negative	29	0.9998	0.8493	positive
5	0.6904	0.4505	negative	30	0.9027	0.6080	positive
6	0.7794	0.9190	negative	31	0.3319	0.1473	positive
		⋮				⋮	

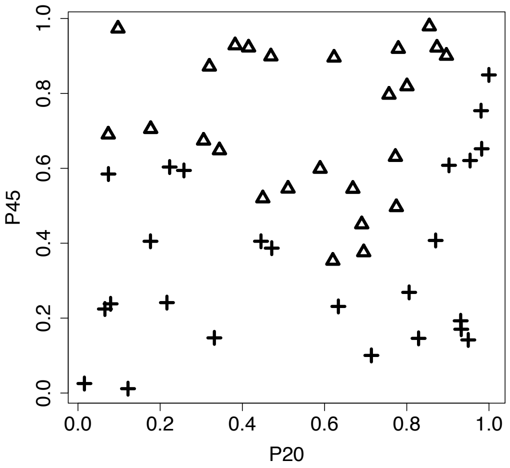


Figure: A scatter plot of the P20 and P45 features from the EEG dataset. *'positive'* images are shown as crosses, and *'negative'* images are shown as triangles.

- A logistic regression model using basis functions is defined as follows:

$$\mathbb{M}_{\mathbf{w}}(\mathbf{d}) = \frac{1}{1 + e^{-\left(\sum_{j=0}^{b} \mathbf{w}[j]\phi_j(\mathbf{d})\right)}} \tag{11}$$

- We will use the following basis functions for the EEG problem:

$$\begin{array}{ll}
\phi_0(\langle \text{P20}, \text{P45} \rangle) = 1 & \phi_4(\langle \text{P20}, \text{P45} \rangle) = \text{P45}^2 \\
\phi_1(\langle \text{P20}, \text{P45} \rangle) = \text{P20} & \phi_5(\langle \text{P20}, \text{P45} \rangle) = \text{P20}^3 \\
\phi_2(\langle \text{P20}, \text{P45} \rangle) = \text{P45} & \phi_6(\langle \text{P20}, \text{P45} \rangle) = \text{P45}^3 \\
\phi_3(\langle \text{P20}, \text{P45} \rangle) = \text{P20}^2 & \phi_7(\langle \text{P20}, \text{P45} \rangle) = \text{P20} \times \text{P45}
\end{array}$$

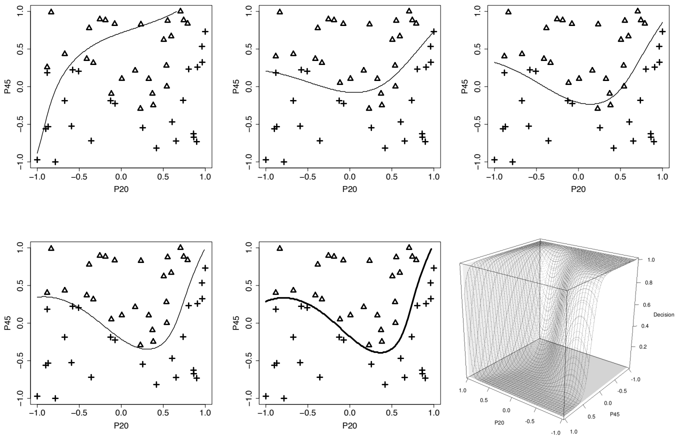
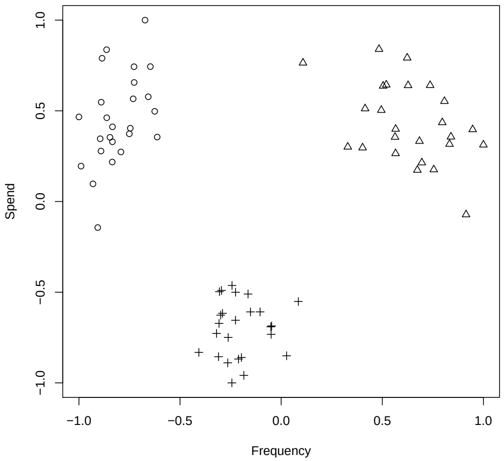


Figure: A selection of the models developed during the gradient descent process for the EEG dataset from Table 6 [55]. The final panel shows the decision surface generated.

Multinomial Logistic Regression

Table: A dataset of customers of a large national retail chain.

ID	Spend	Freq	Type
1	21.6	5.4	single
2	25.7	7.1	single
3	18.9	5.6	single
4	25.7	6.8	single
		⋮	
26	107.9	5.8	business
27	92.9	5.5	business
28	122.6	6.0	business
29	107.7	5.7	business
		⋮	
47	53.2	2.6	family
48	52.4	2.0	family
49	46.1	1.4	family
50	65.3	2.2	family


Spend
Frequency
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

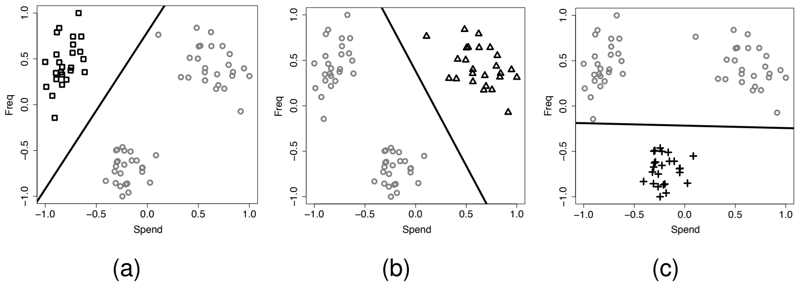


Figure: An illustration of three different **one-versus-all** prediction models for the customer type dataset in Table 7 [61] that has three target levels *'single'* (squares), *'business'* (triangles) and *'family'* (crosses).

- For *r* target feature levels, we build *r* separate logistic regression models $\mathbb{M}_{\mathbf{w_1}}$ to $\mathbb{M}_{\mathbf{w_r}}$:

$$\begin{aligned}
\mathbb{M}_{\mathbf{w_1}}(\mathbf{d}) &= \textit{logistic}(\mathbf{w_1} \cdot \mathbf{d}) \\
\mathbb{M}_{\mathbf{w_2}}(\mathbf{d}) &= \textit{logistic}(\mathbf{w_2} \cdot \mathbf{d}) \\
&\vdots \\
\mathbb{M}_{\mathbf{w_r}}(\mathbf{d}) &= \textit{logistic}(\mathbf{w_r} \cdot \mathbf{d})
\end{aligned} \tag{12}$$

  where $\mathbb{M}_{\mathbf{w_1}}$ to $\mathbb{M}_{\mathbf{w_r}}$ are *r* different one-versus-all logistic regression models, and $\mathbf{w_1}$ to $\mathbf{w_r}$ are *r* different sets of weights.

- To combine the outputs of these different models, we normalize their results using:

$$\mathbb{M}'_{\mathbf{w_k}}(\mathbf{d}) = \frac{\mathbb{M}_{\mathbf{w_k}}(\mathbf{d})}{\sum_{l \in levels(t)} \mathbb{M}_{\mathbf{w}_l}(\mathbf{d})} \tag{13}$$

  where $\mathbb{M}'_{\mathbf{w_k}}(\mathbf{d})$ is a revised, normalized prediction for the one-versus-all model for the target level k.

- The r one-versus-all logistic regression models used are trained in parallel, and the revised model outputs, $\mathbb{M}'_{\mathbf{w_k}}(\mathbf{d})$, are used when calculating the sum of squared errors for each model during the training process.
- This means that the sum of squared errors function is changed slightly to

$$L_2(\mathbb{M}_{\mathbf{w_k}}, \mathcal{D}) = \frac{1}{2}\sum_{i=1}^{n}\left(t_i - \mathbb{M}'_{\mathbf{w_k}}(\mathbf{d}_i\,[1])\right)^2 \qquad (14)$$

- The revised predictions are also used when making predictions for query instances. The predicted level for a query, **q**, is the level associated with the one-versus-all model that outputs the highest result after normalization.
- We can write this as

$$\mathbb{M}(\mathbf{q}) = \underset{l \in levels(t)}{\operatorname{argmax}} \mathbb{M}'_{\mathbf{w}_l}(\mathbf{q}) \tag{15}$$

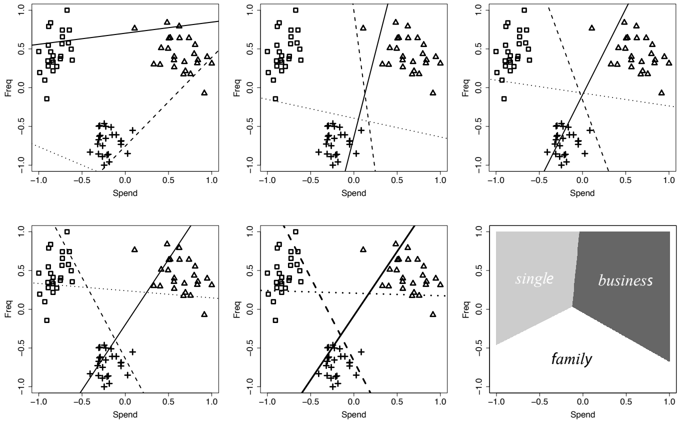
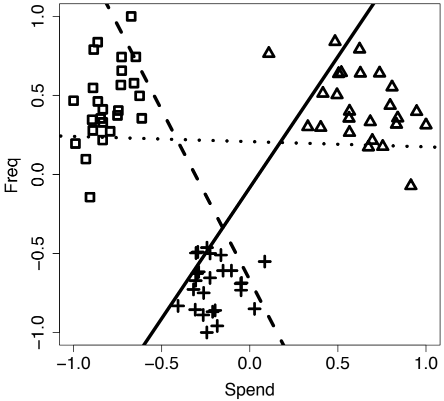


Figure: A selection of the models developed during the gradient descent process for the customer group dataset from Table 7 [61]. Squares represent instances with the *'single'* target level, triangles the *'business'* level and crosses the *'family'* level. (f) illustrates the overall decision boundaries that are learned between the three target levels.



$$\mathbb{M}_{\mathbf{w}_{\textit{'single'}}}(\mathbf{q}) = \textit{Logistic}(0.7993 - 15.9030 \times \textsc{Spend} + 9.5974 \times \textsc{Freq})$$

$$\mathbb{M}_{\mathbf{w}_{\textit{'family'}}}(\mathbf{q}) = \textit{Logistic}(3.6526 + -0.5809 \times \textsc{Spend} - 17.5886 \times \textsc{Freq})$$

$$\mathbb{M}_{\mathbf{w}_{\textit{'business'}}}(\mathbf{q}) = \textit{Logistic}(4.6419 + 14.9401 \times \textsc{Spend} - 6.9457 \times \textsc{Freq})$$

- For a query instance with SPEND $= 25.67$ and FREQ $= 6.12$, which are normalized to SPEND $= -0.7279$ and FREQ $= 0.4789$, the predictions of the individual models would be

$$\begin{aligned}\mathbb{M}_{\mathbf{w}_{\text{'single'}}}(\mathbf{q}) &= \textit{Logistic}(0.7993 - 15.9030 \times (-0.7279) + 9.5974 \times 0.4789)\\ &= 0.9999\\ \mathbb{M}_{\mathbf{w}_{\text{'family'}}}(\mathbf{q}) &= \textit{Logistic}(3.6526 + -0.5809 \times (-0.7279) - 17.5886 \times 0.4789)\\ &= 0.01278\end{aligned}$$

$$\mathbb{M}_{\mathbf{w}_{\text{'business'}}}(\mathbf{q}) = ?$$

- For a query instance with SPEND $= 25.67$ and FREQ $= 6.12$, which are normalized to SPEND $= -0.7279$ and FREQ $= 0.4789$, the predictions of the individual models would be

$$\begin{aligned}\mathbb{M}_{\mathbf{w}_{\textit{'single'}}}(\mathbf{q}) &= \textit{Logistic}(0.7993 - 15.9030 \times (-0.7279) + 9.5974 \times 0.4789)\\ &= 0.9999\\ \mathbb{M}_{\mathbf{w}_{\textit{'family'}}}(\mathbf{q}) &= \textit{Logistic}(3.6526 + -0.5809 \times (-0.7279) - 17.5886 \times 0.4789)\\ &= 0.01278\\ \mathbb{M}_{\mathbf{w}_{\textit{'business'}}}(\mathbf{q}) &= \textit{Logistic}(4.6419 + 14.9401 \times (-0.7279) - 6.9457 \times 0.4789)\\ &= 0.0518\end{aligned}$$

- These predictions would be normalized as follows:

$$\mathbb{M}'_{\mathbf{w}_{\textit{'single'}}}(\mathbf{q}) = \frac{0.9999}{0.9999 + 0.01278 + 0.0518} = 0.9393$$
$$\mathbb{M}'_{\mathbf{w}_{\textit{'family'}}}(\mathbf{q}) = \frac{0.01278}{0.9999 + 0.01278 + 0.0518} = 0.0120$$
$$\mathbb{M}'_{\mathbf{w}_{\textit{'business'}}}(\mathbf{q}) = \frac{0.0518}{0.9999 + 0.01278 + 0.0518} = 0.0487$$

- This means the overall prediction for the query instance is *'single'*, as this gets the highest normalized score.

Support Vector Machines

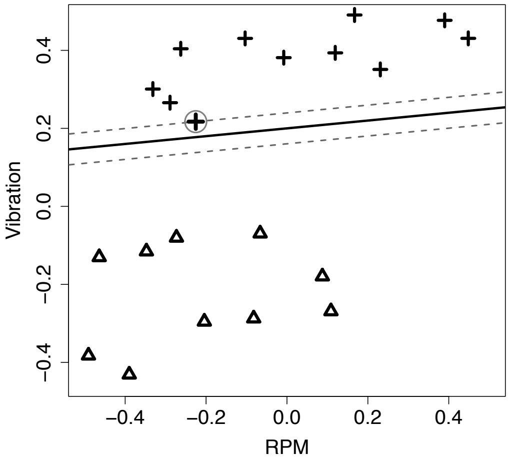


Figure: A small sample of the generators dataset with two features, RPM and VIBRATION, and two target levels, *'good'* (shown as crosses) and *'bad'* (shown as triangles). A decision boundary with a very small margin.

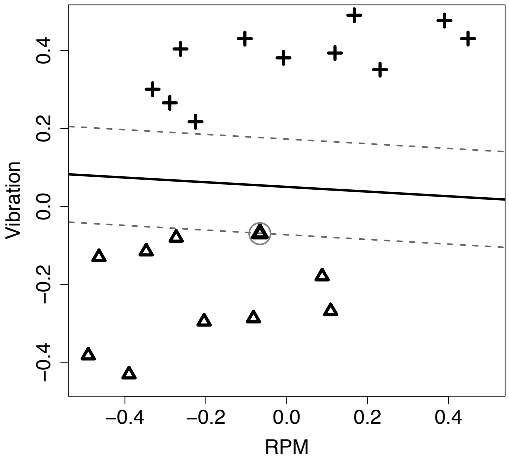


Figure: A small sample of the generators dataset with two features, RPM and VIBRATION, and two target levels, *'good'* (shown as crosses) and *'bad'* (shown as triangles). A decision boundary with a large margin.

- Training a support vector machine involves searching for the decision boundary, or **separating hyperplane**, that leads to the maximum margin as this will best separate the levels of the target feature.
- The instances in a training dataset that fall along the margin extents, and so define the margins, are known as the **support vectors** and define the decision boundary.

- We define the separating hyperplane as follows:

$$w_0 + \mathbf{w} \cdot \mathbf{d} = 0 \tag{16}$$

- For instances above a separating hyperplane

$$w_0 + \mathbf{w} \cdot \mathbf{d} > 0$$

  and for instances below a separating hyperplane

$$w_0 + \mathbf{w} \cdot \mathbf{d} < 0$$

- We build a support vector machine prediction model so that instances with the negative target level result in the model outputting ≤ -1 and instances with the positive target level result in the model outputting $\geq +1$.
- The space between the outputs of -1 and $+1$ allows for the margin.

- A support vector machine model is defined as

$$\mathbb{M}_{\boldsymbol{\alpha},w_0}(\mathbf{q}) = \sum_{i=1}^{s} \left(t_i \times \boldsymbol{\alpha}[i] \times (\mathbf{d}_i \cdot \mathbf{q}) + w_0\right) \tag{17}$$

where

- $\mathbf{q}$ is the set of descriptive features for a query instance;
- $(\mathbf{d}_1, t_1), \ldots, (\mathbf{d}_s, t_s)$ are s support vectors (instances composed of descriptive features and a target feature);
- w_0 is the first weight of the decision boundary;
- and $\boldsymbol{\alpha}$ is a set of parameters determined during the training process (there is a parameter for each support vector $\boldsymbol{\alpha}[1], \ldots, \boldsymbol{\alpha}[s]$).[1]

[1] These parameters are formally known as **Lagrange multipliers**.

- Training a support vector machine is frames as a **constrained quadratic optimization problem**
- This type of problem is defined in terms of:
  1. a set of constraints
  2. an optimization criterion.

- The required **constraints** required by the training process are

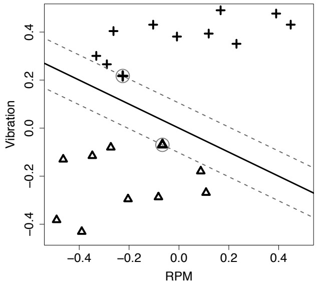
$$w_0 + \mathbf{w} \cdot \mathbf{d} \leq -1 \text{ for } t_i = -1 \tag{18}$$

and:

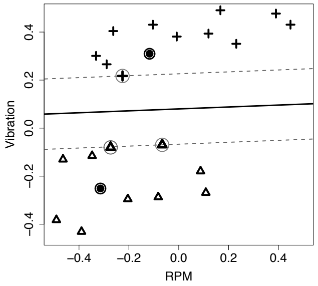
$$w_0 + \mathbf{w} \cdot \mathbf{d} \geq +1 \text{ for } t_i = +1 \tag{19}$$

- We can combine these two constraints into a single constraint (remember t_i is always equal to either -1 or $+1$):

$$t_i \times (w_0 + \mathbf{w} \cdot \mathbf{d}) \geq 1 \tag{20}$$



(a)



(b)

Figure: Different margins that satisfy the constraint in Equation (20)[81]. The instances that define the margin are highlighted in each case. (b) shows the maximum margin and also shows two query instances represented as black dots.

- The **optimization** criterion used is defined in terms of the perpendicular distance from any instance to the decision boundary and is given by

  $$dist(\mathbf{d}) = \frac{w_0 + abs(\mathbf{w} \cdot \mathbf{d})}{||\mathbf{w}||}$$

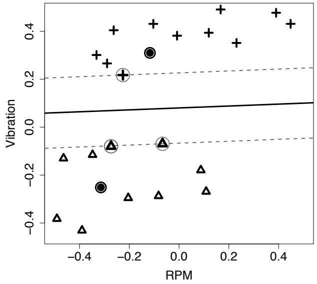
  where $||\mathbf{w}||$ is known as the **Euclidean norm** of **w** and is calculated as

  $$||\mathbf{w}|| = \sqrt{\mathbf{w}[1]^2 + \mathbf{w}[2]^2 + \ldots + \mathbf{w}[m]^2}$$

- For instances along the **margin extents**, $abs(\mathbf{w} \cdot \mathbf{d} + w_0) = 1$.
- So, the distance from any instance along the margin extents to the decision boundary is $\frac{1}{||\mathbf{w}||}$, and because the margin is symmetrical to either side of the decision boundary, the size of the margin is $\frac{2}{||\mathbf{w}||}$.

- The goal when training a support vector machine is
  1. maximize $\frac{2}{||\mathbf{w}||}$
  2. subject to the constraint

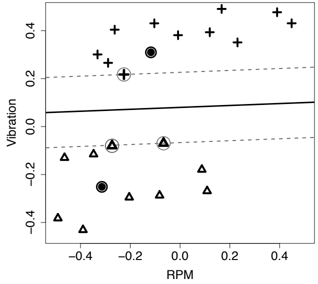
$$t_i \times (w_0 + \mathbf{w} \cdot \mathbf{d}) \geq 1$$



- The optimal decision boundary and associated support vectors for the example we have been following
- In this case *'good'* is the positive level and set to $+1$, and *'faulty'* is the negative level and set to -1.

- The descriptive feature values and target feature values for the support vectors in these cases are
  - $(\langle -0.225, 0.217\rangle, +1)$,
  - $(\langle -0.066, -0.069\rangle, -1)$,
  - $(\langle -0.273, -0.080\rangle, -1)$.
- The value of w_0 is -0.1838,
- The values of the $\boldsymbol{\alpha}$ parameters are

$$\langle 22.056, 6.998, 16.058\rangle.$$



- The plot shows the position of two new query instances for this problem.
- The descriptive feature values for these querys are
  1. $\mathbf{q_1} = \langle -0.314, -0.251 \rangle$
  2. $\mathbf{q_2} = \langle -0.117, 0.31 \rangle$.

- For the first query instance, $\mathbf{q_1} = \langle -0.314, -0.251 \rangle$, the output of the support vector machine model is:

$$\begin{aligned}
&\mathbb{M}_{\boldsymbol{\alpha}, w_0}(\mathbf{q_1})\\
&\quad = (1 \times 23.056 \times ((-0.225 \times -0.314) + (0.217 \times -0.251)) - 0.1838)\\
&\qquad + (-1 \times 6.998 \times ((-0.066 \times -0.314) + (-0.069 \times -0.251)) - 0.1838)\\
&\qquad + (-1 \times 16.058 \times ((-0.273 \times -0.314) + (-0.080 \times -0.251)) - 0.1838\\
&\quad = -2.145
\end{aligned}$$

- The model output is less than -1, so this query is predicted to be a *'faulty'* generator.
- For the second query instance, the model output is 1.592, so this instance is predicted to be a *'good'* generator.

- **Basis functions** can be used with support vector machines to handle data that is not **linearly separable**
- To use basis functions we update Equation (20)[81] to

$$t_i \times (w_0 + \mathbf{w} \cdot \phi(\mathbf{d})) \geq 1 \text{ for all } i \tag{21}$$

where ϕ is a set of basis functions applied to the descriptive features $\mathbf{d}$, and $\mathbf{w}$ is a set of weights containing one weight for each member of ϕ.

- Typically, the number of basis functions in ϕ is larger than the number of descriptive features, so the application of the basis functions moves the data into a higher-dimensional space.
- The expectation is that a linear separating hyperplane will exist in this higher-dimensional space even though it does not in the original feature space.

- The prediction model in this case becomes

$$\mathbb{M}_{\boldsymbol{\alpha},\boldsymbol{\phi},w_0}(\mathbf{q}) = \sum_{i=1}^{s} \left(t_i \times \boldsymbol{\alpha}[i] \times (\phi(\mathbf{d}_i) \cdot \phi(\mathbf{q})) + w_0\right) \qquad (22)$$

- This equation requires a dot product calculation between the result of applying the basis functions to the query instance and to each of the support vectors which is repeated multiple times during the training process.

- A dot product is a computationally expensive operation,
- We can use a clever trick is used to avoid it:
  - the same result obtained by calculating the dot product of the descriptive features of a support vector and a query instance after having applied the basis functions can be obtained by applying a much less costly **kernel function**, *kernel*, to the original descriptive feature values of the support vector and the query.

- The prediction equation becomes

$$\mathbb{M}_{\boldsymbol{\alpha},kernel,w_0}(\mathbf{q}) = \sum_{i=1}^{s} \left(t_i \times \boldsymbol{\alpha}[i] \times kernel\left(\mathbf{d}_i, \mathbf{q}\right) + w_0\right) \quad (23)$$

- A wide range of standard kernel functions can be used with support vector machines including:

Linear kernel	$kernel(\mathbf{d}, \mathbf{q}) = \mathbf{d} \cdot \mathbf{q} + c$ where c is an optional constant
Polynomial kernel	$kernel(\mathbf{d}, \mathbf{q}) = (\mathbf{d} \cdot \mathbf{q} + 1)^p$ where p is the degree of a polynomial function
Gaussian radial basis kernel	$kernel(\mathbf{d}, \mathbf{q}) = \exp(-\gamma\lvert\lvert\mathbf{d} - \mathbf{q}\rvert\rvert^2)$ where γ is a manually chosen tuning parameter