Introduction to Machine Learning

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March 14, 2023

Announcements

- **Individual assignment 2 deadline: 17/03, 23:59**
- **Reading assignment 3 on Transformer models: 20/03**

Overview

Machine Learning

What is Machine Learning?

- What does it mean to learn?
  - Given historical data, we are interested in **predicting** the unseen future.
  - Given unstructured data, we are interested in uncovering **structure** (patterns).
  - Given an environment and a goal, we are interested in **acting** to reach the goal.
- Memorization is not learning, **generalization** is what matters.
- We usually achieve this using an **inductive approach**: by seeing known examples (**train dataset**), we attempt to distill the signal and filter out the noise, in order to predict future examples. We use a left-out slice of the data (**test dataset**) to simulate the future.
- You don't look at your test data! It has to be **unseen**.

Types of ML

- **Supervised learning**: we are given a labelled dataset $\{X, Y\}$, with labels for every data point. Our goal is to learn to **predict** labels for future data points. Examples: regression, classification.
- **Unsupervised learning**: we are given an unlabelled dataset $\{X\}$. Our goal is to learn to **structure** data points in some meaningful way. Examples: clustering, distribution fitting.
- **Reinforcement learning**: we are given an environment and some **agents** acting in it, which have access to a notion of **reward**. Agents seek to take actions in the environment, maximizing the reward. Usually, actions (or sequences thereof) are linked to rewards.
- More: Semi-supervised, Multi-task, Transfer learning, etc.

The components of a probabilistic ML classifier

- A **dataset** and its **feature representation**.
- A **classification function**, or **model**. This model specifies a relationship between inputs and outputs, using parameters (to be learned) and hyperparameters (given by us).
- A **loss function** (also called objective or cost function): something we want to minimize as a proxy for "learning". This function encapsulates what it means to learn for us.
- An algorithm for **optimization**: a way to find good model parameters which minimize the loss function.

Example: The perceptron

- The very beginnings (Rosenblatt 1958), still at the core for the neural model of learning.
- Inspired by a neuron with incoming connections from other neurons that represent features
- We have a **dataset** $\{X, Y\}$, so that $\boldsymbol{x} = \langle x_1, x_2, \ldots, x_d \rangle, y \in \{-1, +1\}, \forall (\boldsymbol{x}, y) \in \{X, Y\}$. We thus have a binary classification problem.
- The **perceptron model** is defined by a linear combination of weights $\langle w_1, w_2, \ldots, w_d \rangle$ and features, plus an optional bias term:

$$a = \left[\sum_{d=1}^{D} w_d x_d \right] + b$$

- *sign* is our **classification function** (positive or negative): does the neuron fire? The bias shifts the decision threshold.

Perceptron loss

- Training a perceptron is online: exemplar by exemplar
- When do we have to adjust the weights?
- We can use the so-called **0/1 loss**.
  $l^{0/1} = \min_{\boldsymbol{w},b} \sum_n \mathbf{1}[y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) < 0]$
- Equivalently, to simplify: $l^{0/1} = \min \sum_n \mathbf{1}[y_n \hat{y} < 0]$
- For each mistaken prediction, penalty of 1
- When the data are linearly separable, the minimum can be zero.
  Why?

Perceptron optimization

- How does the perceptron learn?

$$a = \left[\sum_{d=1}^{D} w_d x_d \right] + b$$

- **Optimization**: it is an online (1 data point at the time) and error-driven algorithm (we want to make no errors). Given a datapoint in the train dataset, *if the perceptron's prediction is correct, do nothing, else*:

$$w_d^t \leftarrow w_d^{t-1} + y x_d$$
$$b^t \leftarrow b^{t-1} + y$$

(y is the label, positive or negative)

Exercise

Exercise: Training a perceptron

Your dataset is the following:
$\{(2,1;-1),(1,2;+1),(3,1;-1),(3,2;-1),(1,3;+1),(2,3;+1)\}$. Assume we use a perceptron without bias term. Also assume we start with random weights: $w_1^{(0)} = 1/2, w_2^{(0)} = -1/2$.

- The first iteration goes as follows:
  1. $a_1 = w_1^{(0)} x_{11} + w_2^{(0)} x_{12} = 1 - 1/2 = 1/2$. $sign(1/2) = +$, thus we have an error and we need to update weights.
  2. Weight update at iteration 1:
  $$w_1^{(1)} \leftarrow w_1^{(0)} + y_1 x_{11} = 1/2 - 2 = -3/2$$
  $$w_2^{(1)} \leftarrow w_2^{(0)} + y_1 x_{12} = -1/2 - 1 = -3/2$$
  3. Proceed to do the same for w_2 and the following data points. Does your perceptron converge to a boundary after one pass on the data? If so, can you draw the boundary?

Exercise

Exercise: Training a perceptron

1. $a_2 = w_1^{(1)} x_{21} + w_2^{(1)} x_{22} = -3/2 - 3 = -4.5$. $sign(-4.5) = -$

$$w_1^{(2)} \leftarrow w_1^{(1)} + y_1 x_{11} = -3/2 + 1 = -1/2$$
$$w_2^{(2)} \leftarrow w_2^{(1)} + y_1 x_{12} = -3/2 + 2 = 1/2$$

2. $a_3 = w_1^{(1)} x_{31} + w_2^{(1)} x_{32} = -3/2 + 1/2 = -1$. $sign(-1) = -$
3. $a_4 = w_1^{(1)} x_{41} + w_2^{(1)} x_{42} = -3/2 + 1 = -1/2$. $sign(-1/2) = -$
4. $a_5 = w_1^{(1)} x_{51} + w_2^{(1)} x_{52} = -1/2 + 3/2 = 1$. $sign(1) = +$
5. $a_6 = w_1^{(1)} x_{61} + w_2^{(1)} x_{62} = -2/2 + 3/2 = 1/2$. $sign(1/2) = +$

In summary

- Some properties of the perceptron include:
  1. **It always converges if the data points are linearly separable**.
  2. It is unable to distinguish among decision boundaries.
  3. The linear model it embeds computes **a projection of every feature** x_d onto the vector $\boldsymbol{w}$. This means that we basically order the projected features on a line, sum them up and check if they are above or below a threshold!
  4. It is unable to go beyond linearly separable data (infamous XOR problem). Extensions include: 'stacking up' perceptrons (**neural networks**) and doing feature maps (**kernel methods**).
  5. See HD, ch. 4 for more.

Key concepts: Generalization

- We have a loss function l and a dataset $\{X, Y\}$. We take a probabilistic view and state that we *assume* the existence of a data generating distribution $\mathcal{D}$ over data pairs (x, y), giving probabilities to pairs of data points. We then learn a function f that minimizes the loss for our data points, in view of generalizing to new data points under $\mathcal{D}$.
- We would like to learn to minimize the **expected loss** ϵ over $\mathcal{D}$:

$$\epsilon := \mathbb{E}_{(x,y)\sim\mathcal{D}}\Big[l(y, f(x))\Big] = \sum_{(x,y)} \mathcal{D}(x, y) l(y, f(x))$$

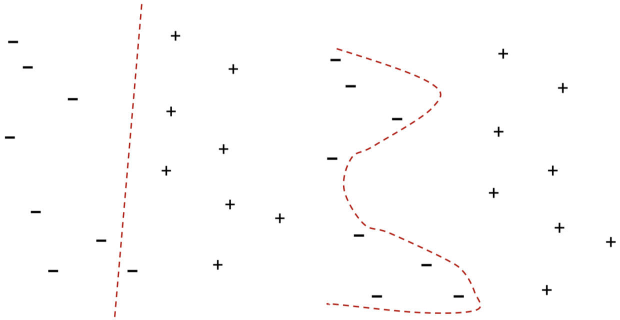
- But we do not know $\mathcal{D}$!
- Instead, we compute the **training error** $\hat{\epsilon}$ assuming it approximates ϵ:

$$\hat{\epsilon} := \frac{1}{N} \sum_{n=1}^{N} l(y_n, f(x_n))$$

- Which means we assume $\mathcal{D}$ to be uniform over our training examples and zero anywhere else. That is: **independent, uniformly and identically distributed**.

Key concepts: Underfitting and overfitting

- **Underfitting**: "you had an opportunity to learn something but did not". **Overfitting**: "you pay too much attention to the idiosyncracies of the data, and are not able to generalize well." HD, ch. 2.



Key concepts: Underfitting and overfitting

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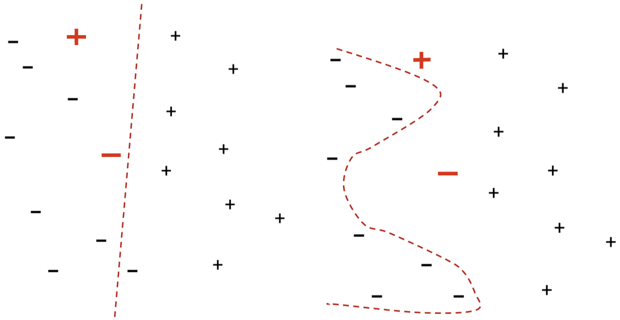
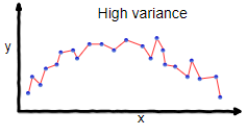
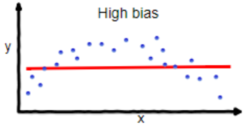


Key concepts: Underfitting and overfitting

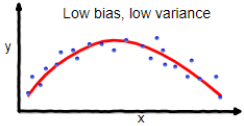
- Also referred to as **Bias-variance trade-off**.
- Note: this theory seems not to apply to deep learning! Belkin, Mikhail, Daniel Hsu, Siyuan Ma, and Soumik Mandal. 2019. "Reconciling Modern Machine-Learning Practice and the Classical Bias–Variance Trade-Off." Proceedings of the National Academy of Sciences 116 (32): 15849–54. `https://doi.org/10.1073/pnas.1903070116`.



overfitting



underfitting



Good balance

Key concepts: Optimization

- Every **parametric model** expresses a set of parameters, which we need to tune during learning. E.g., word2vec.
- **Non-parametric models** instead, use the whole dataset as parameters. E.g., k-NN (nearest neighbours), as we will see later on.
- **Regularization**: adding constraints to parameters to avoid overfitting.
- **Hyperparameters**: not learned with the model/optimization. We can still use the data to find good values. E.g., **cross-validation**: train different models over a range of hyperparameter combinations, and pick the best. We use a third slice of the dataset for this: the **validation (or development) set**.

Linear Regression

Linear models for regression

- We have a **dataset** $\{X, Y\}$, so that $\boldsymbol{x} = \langle x_1, x_2, \ldots, x_d \rangle, y \in \mathbb{R}$, $\forall(\boldsymbol{x}, y) \in \{X, Y\}$. We thus have a regression problem.
- Examples: predict house prices, predict height of persons.
- The **model** is **a linear, weighted combination of the inputs**. In general:

$$\hat{y} = b + \sum_{d=1}^{D} w_d x_d$$

- y is the true value, $\hat{y}$ is the predicted value from the model.
- I will put the intercept b in the summation as w_0 by adding an $x_0 = 1$, and use matrix notation (in bold):

$$\hat{y} = \sum_{d=0}^{D} w_d x_d$$

$$\hat{y} = \boldsymbol{X}\boldsymbol{w}$$

Loss functions: Convexity

- With the perceptron, we used the so-called **0/1 loss**.
  $l^{0/1} = \min_{\boldsymbol{w},b} \sum_n \mathbf{1}[y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) < 0]$
- Equivalently, to simplify: $l^{0/1} = \min \sum_n \mathbf{1}[y_n \hat{y} < 0]$
- Unfortunately, the perceptron's learning algorithm is feasible only if the data points are linearly separable, i.e. if the minimum of $l^{0/1}$ is zero. This is rarely the case in practice. *Question: what happens if we use the perceptron on a dataset which is not linearly separable?*
- A popular alternative is to choose less exact but easier to work with loss functions. In particular, we pick from **convex functions**, so that we can use techniques from calculus.

Convexity

- **A function is convex if, equivalently: its second derivative is always positive or any chord of the function lies above it.**

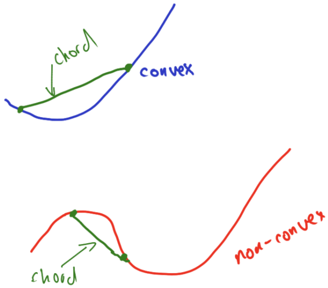


Figure 7.3: plot of convex and non-convex functions with two chords each

Credit: HD, ch. 7.

Loss functions for linear regression

- There is a variety of loss functions which are convex or semi-convex. There are several options for linear regression. For example:
  1. **Mean Squared Error (MSE)**: $l^{MSE} = \min \sum_n (y_n - \hat{y})^2$
  2. Mean Absolute Error (MAE): $l^{MAE} = \min \sum_n |y_n - \hat{y}|$
  3. Hinge: $l^{hin} = \min \sum_n max\{0, 1 - y_n \hat{y}\}$
- They vary on how they deal with erroneous predictions (e.g., MSE is very sensitive to them) and with confident correct predictions (e.g., ignore them with Hinge).
- They are **differentiable or semi-differentiable**.

Closed-form solution for MSE Linear regression

- Let us pick MSE. In this particular case, we can derive a closed-form solution via calculus.
- What we have, in matrix notation:

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{w}$$

$$\mathcal{L} = \frac{1}{2}||\hat{\boldsymbol{y}} - \boldsymbol{y}||^2$$

$$\underbrace{\begin{bmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,D} \\ x_{2,1} & x_{2,2} & \dots & x_{2,D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N,1} & x_{N,2} & \dots & x_{N,D} \end{bmatrix}}_{\mathbf{X}} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix}}_{\boldsymbol{w}} = \underbrace{\begin{bmatrix} \sum_d x_{1,d} w_d \\ \sum_d x_{2,d} w_d \\ \vdots \\ \sum_d x_{N,d} w_d \end{bmatrix}}_{\hat{\mathbf{Y}}} \approx \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\hat{\mathbf{Y}}} \tag{7.29}$$

Credit: HD, ch. 7.

Closed-form solution for MSE Linear regression

- We can express the loss as follows:

$$\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) = \frac{1}{2}||\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}||^2$$

- We use calculus to minimize the loss by setting its derivative to zero:

$$\begin{aligned} \bigtriangledown_{\boldsymbol{w}}\mathcal{L}(\boldsymbol{w}) &= \boldsymbol{X}^T\Big(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\Big) = 0 \\ \boldsymbol{w} &= \Big(\boldsymbol{X}^T\boldsymbol{X}\Big)^{-1}\boldsymbol{X}^T\boldsymbol{y} \end{aligned}$$

- This is an exact, but costly solution. Complexity: $\mathcal{O}\Big(D^3 + D^2N\Big)$, with D number of features and N number of data points.

Regularization

- Left unconstrained, MSE can easily lead to a case of **overfitting**, e.g. by paying too much attention to **outliers** (*why?*).
- Regularization is a way to compensate for this, by constraining weights to be small. It puts a premium on learning simple functions, by moving the model towards being more biased (*why?*).
- Examples of regularizers:
  - L_2-norm (Ridge): $\lambda||\boldsymbol{w}||^2$
  - L_1-norm (Lasso): $\lambda|\boldsymbol{w}|$
- λ is a hyperparameter to control the intensity of the regularization.
  - Independent of the model and data
  - Penalty for exactly fitting the data

Closed-form solution with regularization

- We can express the loss as follows:

$$\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) = \frac{1}{2}||\boldsymbol{X}\boldsymbol{w} - \hat{\boldsymbol{y}}||^2 + \frac{\lambda}{2}||\boldsymbol{w}||^2$$

- We use calculus to minimize the loss by setting its derivative to zero:

$$\bigtriangledown_{\boldsymbol{w}}|\mathcal{L}(\boldsymbol{w}) = \boldsymbol{X}^T\Big(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\Big) + \lambda\boldsymbol{w} = 0$$

$$\boldsymbol{w} = \Big(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}_D\Big)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

- It still works as long as the regularization term is also convex

(Stochastic) Gradient Descent (SGD)

- There is not always a closed-form solution
- General-purpose method to find *a* minimum of differentiable functions. The bread and butter of deep learning.
- The **gradient of a function** $\bigtriangledown_w f$ is the vector consisting of the partial derivatives of this function w.r.t. each input coordinate:

$$\bigtriangledown_w f = \left\langle \frac{\partial f}{\partial w_1}, \frac{\partial f}{\partial w_1}, \ldots, \frac{\partial f}{\partial w_D} \right\rangle$$

- SGD defined an iterative approach to reach a minimum of a function by **gradual update steps**:

$$\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{w}^{(t-1)} - \eta \bigtriangledown_w f$$

- η (eta) is called the **learning rate**. We refer to **stochastic** GD when we use one (or few) data point(s) at the time.

Stochastic Gradient Descent (SGD)

- SGD defined an iterative approach to reach a minimum of a function by **gradual update steps**:

$$\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{w}^{(t-1)} - \eta \bigtriangledown_{w} f$$

$$w_1^{(t)} \leftarrow w_1^{(t-1)} - \eta \frac{\partial f}{\partial w_1}$$

Algorithm 21 $\textsc{GradientDescent}(\mathcal{F}, K, \eta_1, \ldots)$

```
z^(0) ← ⟨0, 0, ..., 0⟩                  // initialize variable we are optimizing
for k = 1 ... K do
    g^(k) ← ∇_z F |_{z^(k-1)}           // compute gradient at current location
    z^(k) ← z^(k-1) − η^(k) g^(k)       // take a step down the gradient
end for
return z^(K)
```

Credit: HD, ch. 7.

Stochastic Gradient Descent (SGD)

- SGD defined an iterative approach to reach a minimum of a function by **gradual update steps**:

$$\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{w}^{(t-1)} - \eta \bigtriangledown_{w} f$$

For a single scalar:

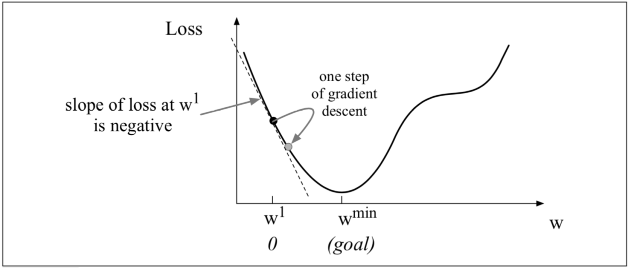


Figure 5.3 The first step in iteratively finding the minimum of this loss function, by moving w in the reverse direction from the slope of the function. Since the slope is negative, we need to move w in a positive direction, to the right. Here superscripts are used for learning steps, so w^1 means the initial value of w (which is 0), w^2 at the second step, and so on.

Credit: J&M, ch. 5.

Stochastic Gradient Descent (SGD)

- SGD defined an iterative approach to reach a minimum of a function by **gradual update steps**:

$$\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{w}^{(t-1)} - \eta \bigtriangledown_{w} f$$

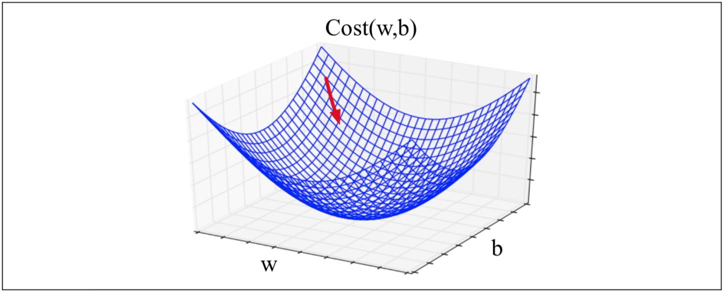


Figure 5.4 Visualization of the gradient vector in two dimensions *w* and *b*.

Credit: J&M, ch. 5.

Stochastic Gradient Descent (SGD)

- SGD defined an iterative approach to reach a minimum of a function by **gradual update steps**:

$$\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{w}^{(t-1)} - \eta \bigtriangledown_{w} f$$

- η (eta) is called the **learning rate**: this is crucial for convergence.

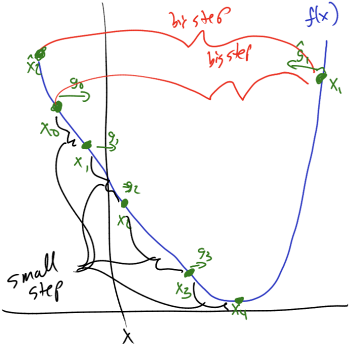
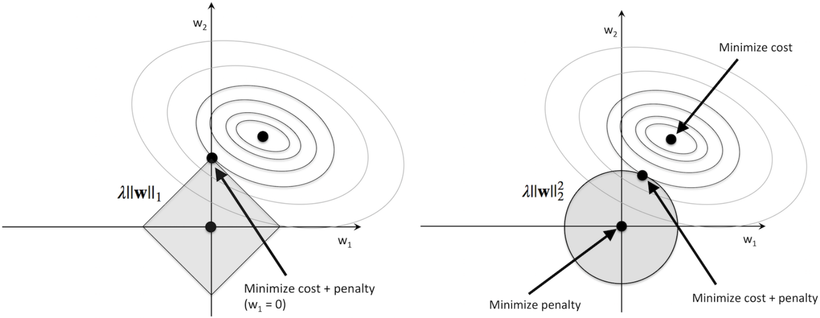


Figure 7.7: good and bad step sizes

Regularization and SGD



gray area = regularization constraint

Notation note: $||\boldsymbol{w}||_p = \left(\sum_d |\boldsymbol{w_d}|^p\right)^{\frac{1}{p}}$.
I have implied so far: $||\boldsymbol{w}||^2 = ||\boldsymbol{w}||_2^2$ and $|\boldsymbol{w}| = ||\boldsymbol{w}||_1$.

`http://rasbt.github.io/mlxtend/user_guide/general_concepts/regularization-linear`.

Putting everything together (SGD)

- SGD:

$$\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{w}^{(t-1)} - \eta \bigtriangledown_w f$$

- Loss for linear regression with Mean Absolute Error and L_2:

$$\mathcal{L}(\boldsymbol{w}) = \frac{1}{2}||\boldsymbol{X}\boldsymbol{w} - \hat{\boldsymbol{y}}||^2 + \frac{\lambda}{2}||\boldsymbol{w}||^2$$

- Regularized SGD for linear regression with MAE and L_2:

$$\boldsymbol{w}^{(t)} \leftarrow \boldsymbol{w}^{(t-1)} - \eta \bigtriangledown_w \mathcal{L}$$

- Same, for datapoint x_z and for weight w_1:

$$w_1^{(t)} \leftarrow w_1^{(t-1)} - \eta \frac{x_{z1} y_z}{x_{z1}^2 + \lambda}$$

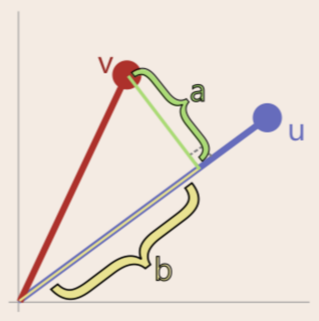
- Often, we feed data to SGD in **batches** (e.g., a few tens or hundreds data points at the time). Data size issue

Notes

Notes

Extras

Dot products



- Suppose $||\boldsymbol{u}|| = 1$, i.e. we have a unit vector (of length one, this makes the point easier to see).
- We can think of $\boldsymbol{v}$ as the sum of two components, one parallel (b) and another perpendicular (a) to $\boldsymbol{u}$.
- The dot product $\boldsymbol{u} \cdot \boldsymbol{v}$ gives you b, the projection of $\boldsymbol{v}$ onto $\boldsymbol{u}$ over all their dimensions.

Dot products in the perceptron model

F

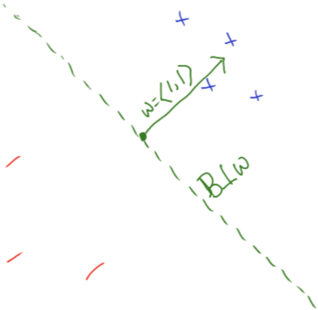


Figure 4.6: picture of data points with hyperplane and weight vector

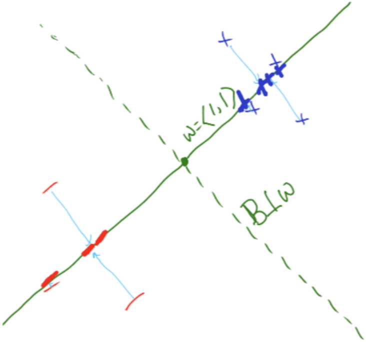


Figure 4.7: The same picture as before, but with projections onto weight vector; then, below, those points along a one-dimensional axis with zero marked.

Credit: HD, ch. 4.

Full derivation for linear regression

- Closed-form, with MSE loss and L_2 regularization:

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{w}) &= \frac{1}{2}||\boldsymbol{X}\boldsymbol{w} - \hat{\boldsymbol{y}}||^2 + \frac{\lambda}{2}||\boldsymbol{w}||^2 \\
\nabla_w \mathcal{L}(\boldsymbol{w}) &= \boldsymbol{X}^T\Big(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\Big) + \lambda \boldsymbol{w} \\
\text{(put equal to zero)} \rightarrow \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} + \lambda\boldsymbol{w} &= \boldsymbol{X}^T\boldsymbol{y} \\
\Big(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}\Big)\boldsymbol{w} &= \boldsymbol{X}^T\boldsymbol{y} \\
\boldsymbol{w} &= \Big(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}\Big)^{-1}\boldsymbol{X}^T\boldsymbol{y}
\end{aligned}
$$