ML Workshop

Supervised Setting

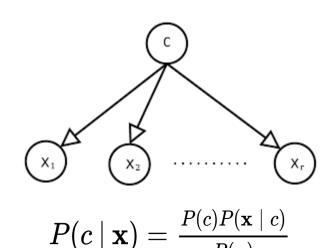
Presented by Rachel Redberg

Whirlwind Overview

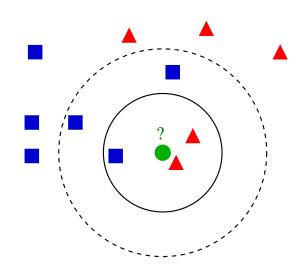
Decision Trees

is age > 9.5? Survived 0.73 36% is sibsp > 2.5? died 0.05 2% survived 0.89 2%

Naive Bayes



k-NN



Supervised Learning

Given a set of labeled training examples (x_i, y_i) , learn a function f mapping input to output:

$$\mathbf{f}(x_i) pprox y_i$$

Classification:

Regression:
$$y_i \in \{0,1,\ldots,n\}$$
 $y_i \in \mathbf{R}$

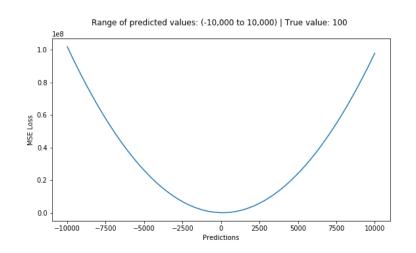
Oftentimes, learning a model in the supervised setting involves minimizing a loss function $L(y, \hat{y})$ which penalizes prediction error:

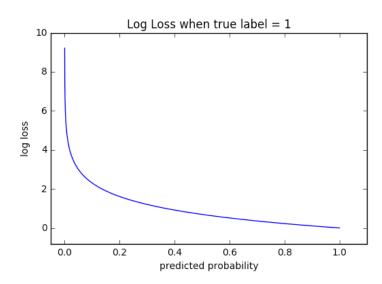
Mean Squared Error (MSE):

Log

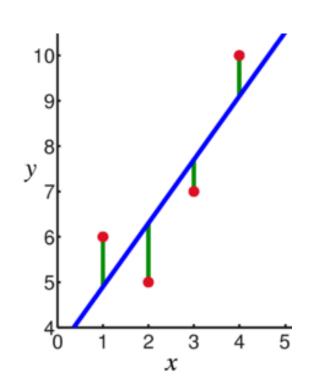
loss:

$$rac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 - (y \log(p) + (1-y) \log(1-p))$$





Linear Regression (Least Squares)



Prediction:

$$y_i = f(x_i) = x_i^T eta + eta_0$$

Learning:

$$\beta = \operatorname{argmin}_b \sum_{i=1}^n (y_i - x_i^T b)^2$$
$$= \operatorname{argmin}_b (y - Xb)^T (y - Xb)$$

Linear Regression (Least Squares)

Closed form solution:

$$eta = (X^T X)^{-1} X^T y$$

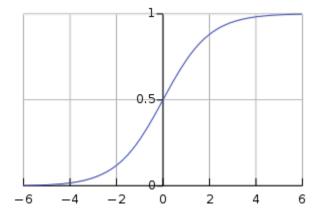
For
$$f(\beta)=(y-X\beta)^T(y-X\beta)$$
 $\partial f/\partial \beta=0$, set β .

and solve for

Logistic Regression

Models the probability of a binary independent variable as a function of multiple independent variables:

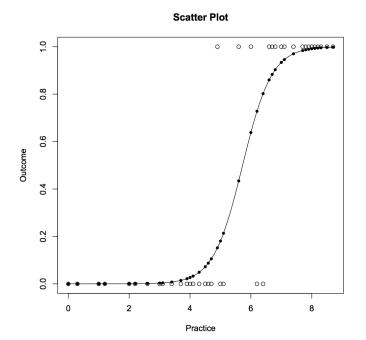
$$P(Y=1|X=x)=rac{e^{eta_0+eta_1x_1+\ldots+eta_nx_n}}{rac{1+e^{eta_0+eta_1x_1+\ldots+eta_nx_n}}{1+e^{eta_0+eta_1x_1+\ldots+eta_nx_n}}}=\sigma(x^Teta+eta_0)$$



$$x,eta\in\mathbb{R}^n,\ Y\in\{0,1\},\ \sigma(x)=rac{e^x}{1+e^x}$$

Logistic Regression

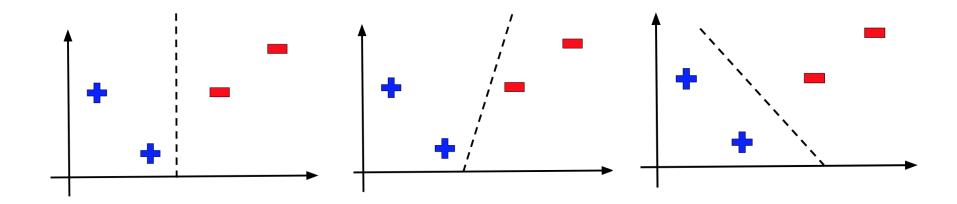
How to solve for beta? Define a likelihood function and maximize it with gradient descent. Assuming observations are independent, the likelihood is given by



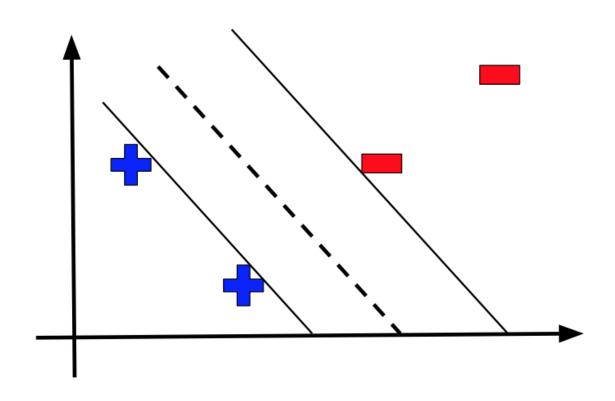
$$egin{aligned} \mathcal{L}ig(eta,eta_0ig) &= \prod\limits_{i=1}^N \Pr(Y=y_i \mid X=x_i) \ &= \prod\limits_{i=1}^N p(x_i)^{y_i} (1-p(x_i))^{1-y_i} \ \end{aligned}$$
 for $p(x;eta,eta_0) = rac{e^{eta 0 + x^Teta}}{1 + e^{eta 0 + x^Teta}}$

Support Vector Machines (SVM)

Given a set of linearly separable training data, how to compute a decision boundary? Which is the best separator/hyperplane?



Widest Margin Approach (SVM)



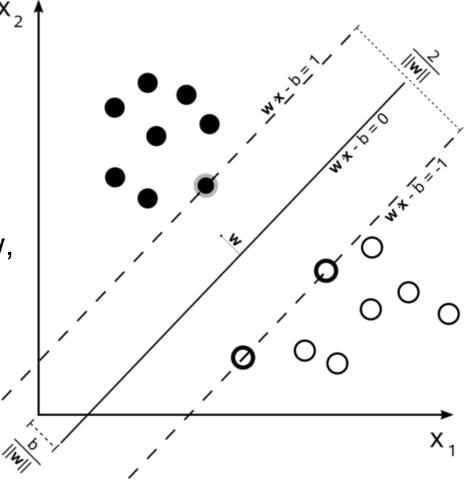
Decision Rule:

If $w^Tx + b \ge 1$ ther

If $w^Tx + b \le -1$ then O.

 w^Tx is the projection of x onto w, b is the bias.

Points on the margin $(w^Tx + b = \pm 1)$ are called support vectors.

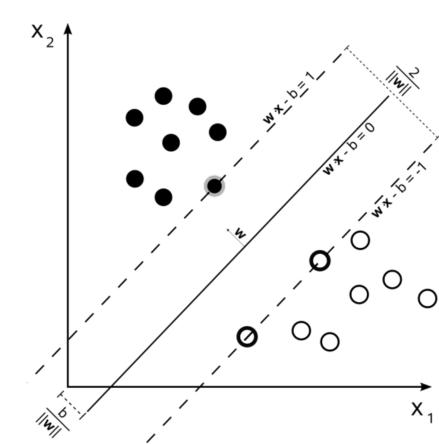


Maximize the margin

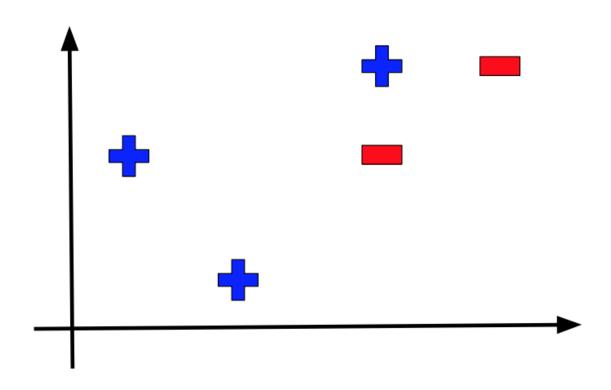
SVM:

$$\min rac{1}{2} ||w||^2$$

s.t. $y_i(w^Tx_i+b)\geq 1 \ orall i$



What if the data isn't linearly separable?

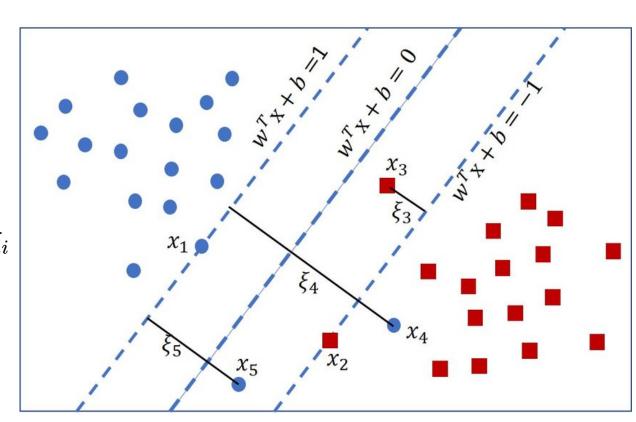


Slack variables

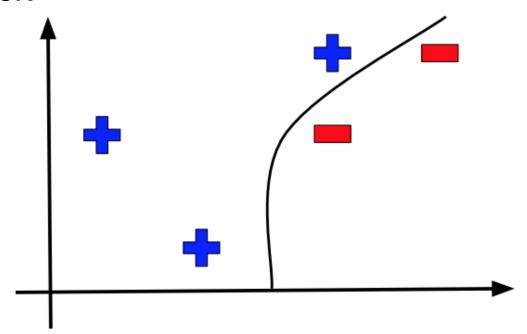
Soft-margin SVM:

$$egin{aligned} \minrac{1}{2}||w||^2 + C\sum_i \xi_i \ ext{s.t.} \ y_i(w^Tx_i+b) & \geq 1-\xi_i \end{aligned}$$

$$\xi_i \geq 0$$



Kernel Trick



Apply a transformation ϕ :

$$K(x_i, x_j) = \phi(x_i)\phi(x_j)$$
 is a kernel function

Primal form of SVM:

$$\min rac{1}{2}||w||^2$$
 st. $y_i(\mathbf{w}.\mathbf{x}_i+b)\geq 1$

Dual form of SVM:

$$\max \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i} \sum_{j} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i} \cdot \mathbf{x}_{j}$$

$$st. \qquad \sum_{i} \alpha_{i} y_{i} = 0$$

$$\alpha_{i} \geq 0$$

We can apply a transformation ϕ

$$\max \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i} \sum_{j} \alpha_{i} \alpha_{j} y_{i} y_{j} \phi(\mathbf{x}_{i}).\phi(\mathbf{x}_{j})$$

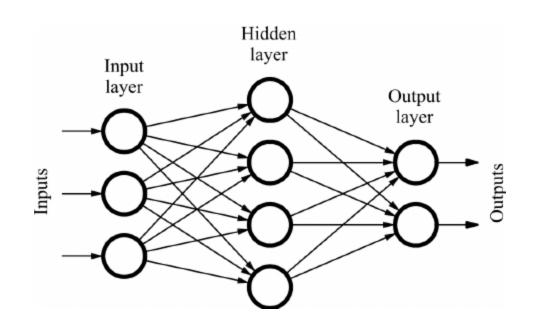
$$st. \qquad \sum_{i} \alpha_{i} y_{i} = 0$$

$$\alpha_{i} \geq 0$$

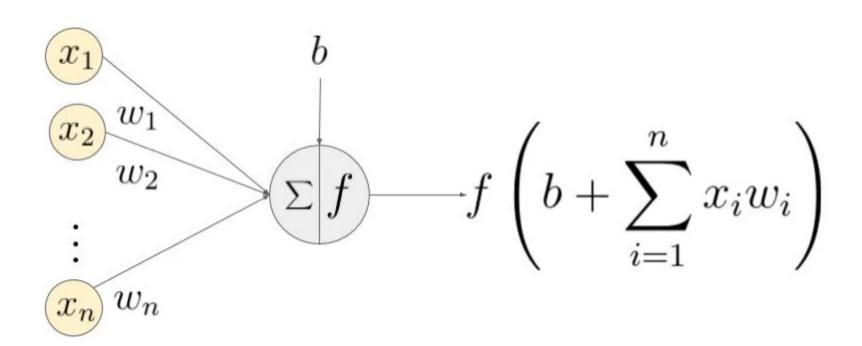
Examples of kernels:

$$egin{aligned} \mathcal{K}(\mathbf{x}_i,\mathbf{x}_j) &= (\mathbf{x}_i.\mathbf{x}_j+1)^n \ \mathcal{K}(\mathbf{x}_i,\mathbf{x}_j) &= e^{-rac{||\mathbf{x}_i-\mathbf{x}_j+1||}{\sigma}} \end{aligned}$$

Deep Learning (Feedforward Neural Network)



A closer look...

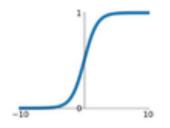


Activation Functions

Derivatives

Sigmoid

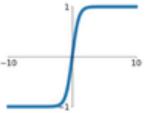
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



$\sigma(x)(1-\sigma(x))$

tanh

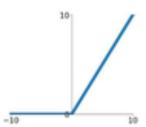
tanh(x)



$1-\sigma(x)^2$

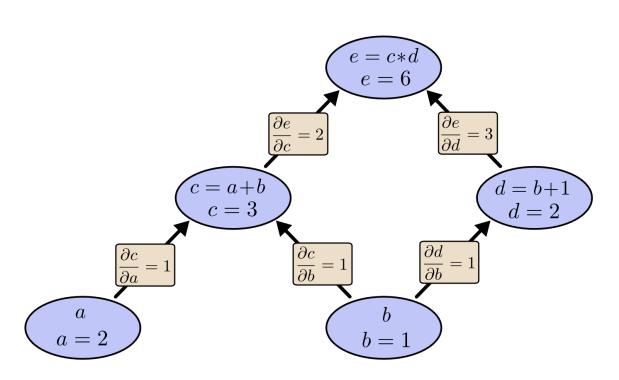
ReLU

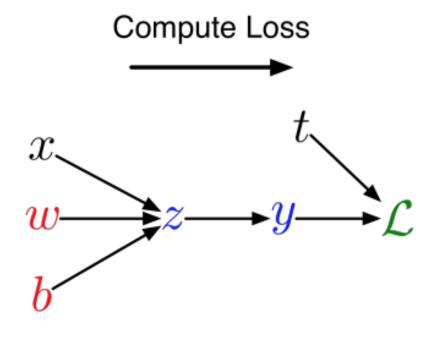
 $\max(0, x)$



0 if
$$x \le 0, 1$$
 if $x > 0$

Backpropagation (Computational Graphs)





Compute Derivatives

x is the input,
w is the weight,
b is the bias,
y is the predicted output, and
t is the true value

Computing the loss:

$$z = wx + b$$

$$y = \sigma(z)$$

$$\mathcal{L}=\frac{1}{2}(y-t)^2$$

Computing the derivatives:

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} = y - t$$

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\mathbf{L}}$$
.

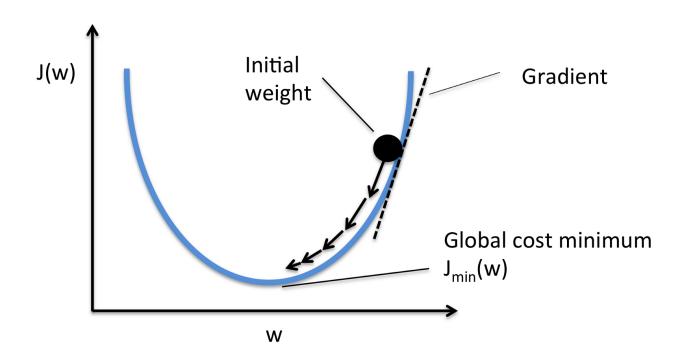
$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} \cdot \sigma'(z)$$

$$\frac{\mathrm{d}y}{\mathrm{d}\mathcal{L}} \cdot y$$

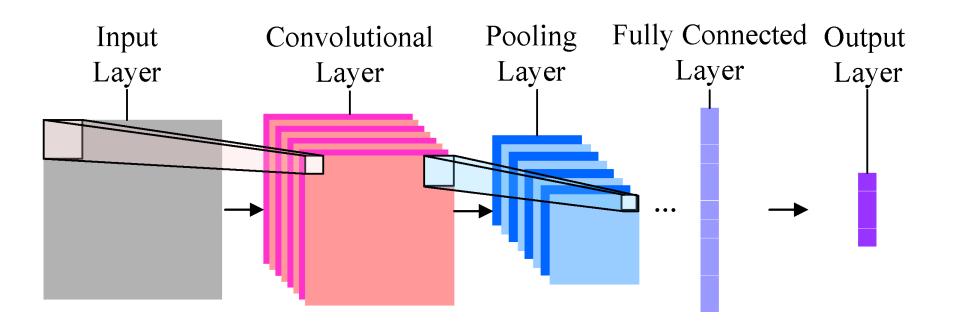
$$\frac{\partial \mathcal{L}}{\partial w} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z} \cdot x$$
$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}$$

Gradient Descent

Update rule:
$$w_j^{(t+1)} = w_j^{(t)} \ - \eta rac{\partial}{\partial w_j} J(w)$$



Convolutional Neural Network



Convolutional neural networks

- Often used for image processing tasks.
- Inspired by biological processes in the visual cortex.
- Exploit statistical patterns in the data:
 - Shared weights
 - Translation invariance
- Network learns filters which extract a particular pattern (e.g. edges, textures) from the image.
- Hierarchical structure: complex patterns are built out of simpler ones.

CNN Layers

Convolutional Layer:

Convolutional kernels are matrices of a given size (e.g., 3 x 3) which are "convolved" with the image to extract features.

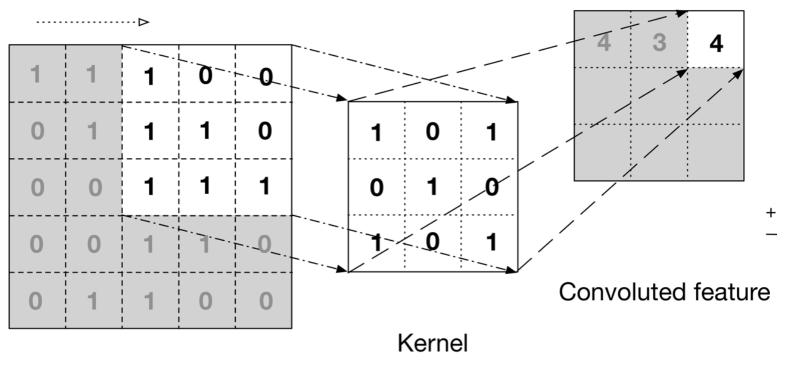
(Max) Pooling Layer:

Pooling layers reduce the dimensionality of the previous layer's output ("downsample") by combining the output of non-overlapping sub-regions of the original representation.

Fully Connected Layer:

Typically need to "flatten" the matrix and feed it into a fully-connected layer to aggregate output from the convolutional/pooling layers, for the final classification.

Convolutional Layer



Input data

Max Pooling Layer

12	20	30	0			
8	12	2	0	2×2 Max-Pool	20	30
34	70	37	4		112	37
112	100	25	12			

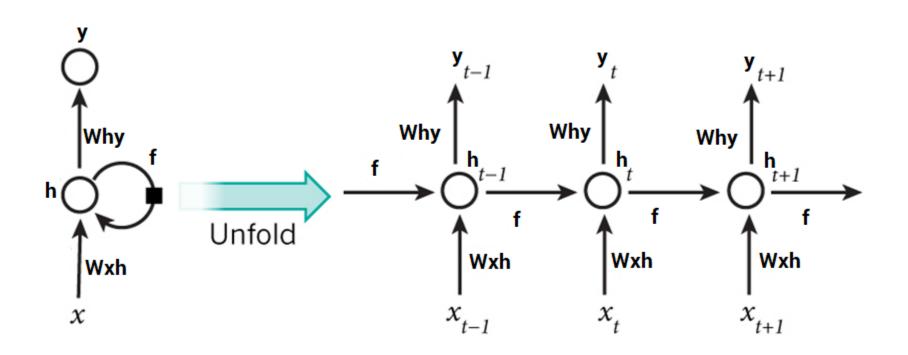
Flatten Matrix

1	1	0
4	2	1
0	2	1



1
1
0
4
2
1
0
2

Recurrent Neural Networks



Recurrent Neural Networks

- Networks with loops to "remember" information from a previous time step.
- Useful for tasks that involve sequences of data:
 - Language models (character-level, word-level), translation, speech recognition, speech-to-text,
 handwritten character generation, time series forecasting, etc.
- Previous information might be helpful for the present task:
 - E.g., in video captioning, use information from previous video frames to make a prediction related to the current frame.
- Issues with vanishing/exploding gradient:
 - Long short-term memory (LSTM) architecture introduces "forget" gates to learn long-term dependencies; decide which values to forget and which to update.

References

Slides are based on:

https://en.wikipedia.org/wiki/Decision_tree_learning

https://www.mdpi.com/1099-4300/19/6/247

https://www.analyticsvidhya.com/blog/2018/03/introduction-k-neighbours-algorithm-clustering/

https://heartbeat.fritz.ai/5-regression-loss-functions-all-machine-learners-should-know-4fb140e9d4b0

https://ml-cheatsheet.readthedocs.io/en/latest/loss functions.html

https://en.wikipedia.org/wiki/Linear regression

https://www.kdnuggets.com/2017/10/learn-generalized-linear-models-glm-r.html/2

https://www.researchgate.net/figure/SVM-with-soft-margin-kernel-with-different-cases-of-slack-variables fig2 327015448

https://iq.opengenus.org/feed-forward-neural-networks/

https://www.learnopencv.com/understanding-feedforward-neural-networks/

https://sebastianraschka.com/fag/docs/relu-derivative.html

https://www.quora.com/Why-is-ReLU-the-most-common-activation-function-used-in-neural-networks

https://colah.github.io/posts/2015-08-Backprop/

http://www.cs.toronto.edu/~rgrosse/courses/csc321 2017/slides/lec6.pdf

https://www.analyticsvidhya.com/blog/2017/12/introduction-to-recurrent-neural-networks/

https://rubikscode.net/2018/02/26/introduction-to-convolutional-neural-networks/

https://www.superdatascience.com/the-ultimate-guide-to-convolutional-neural-networks-cnn/

http://www.davidsbatista.net/blog/2018/03/31/SentenceClassificationConvNets/

https://www.analyticsvidhya.com/blog/2017/12/introduction-to-recurrent-neural-networks/

https://hackernoon.com/gradient-descent-aynk-7cbe95a778da

Arlei Silva's IGERT bootcamp presentation