Linear Models (Linear Regression, Logistic Regression, Softmax)

- Supervised learning
 - What, why, how
 - Machinelearning learns mathematical models from data
 - What is supervised learning and the model
 - \blacksquare D = (x,y). X = input/features. Y = target (classicication or regression)
 - Target function h(x) = f(x)
 - error in and out and Error functions
 - Least squares
 - Capture the problem we consider (FBI)...
 - Linear models:
 - Linear regression: real number. h(x) = w^t x
 - Linear classification: binary decision. $h(x) = sign(w^t x)$
 - Logistic regression: Probability of class. $h(x) = o (w^{t} x)$
- Linear Regression,
 - What does it. Example, house price vs size
 - \circ h(x) = w^t x
 - Error + typical not on w0
 - Minimize (why good idea, and how -v-)
- Optimization / gradient descent
 - Minimize Ein
 - Formel, Compute, Solve for diff = 0
 - Global or local minimizer we found?
 - Convexity
 - (what) What is convex
 - (why) If tangent is below the function (bowl) -> diff f(x) = 0 is a global minimizer
 - (why) why do we want this)
 - (how) tjek doubelt diff er >= 0 for alle x. $f(x) = x^2 f'(x) = 2 >= 0$.

Affine Functions:

$$f(x) = w^{\mathsf{T}}x + c, \quad H_f(x) = 0$$

Quadratic Functions:

$$f(x) = \frac{1}{2}x^{\mathsf{T}}Ax + b^{\mathsf{T}}x + c, \quad H_f(x) = A$$

Iff A is positive semidefinite

$$E_{in}(w) = \frac{1}{n} \sum_{(x,y) \in D} (w^{\mathsf{T}} x - y)^2 = \frac{1}{n} (Xw - y)^{\mathsf{T}} (Xw - y)$$

$$= w^{\intercal}(X^{\intercal}X)w + (-2y^{\intercal}X)^{\intercal}w + y^{\intercal}y$$

1/n died mistakenly, luckily it does not matter)

Convexity of Linear Regression

Quadratic Functions: $f(x) = \frac{1}{2}x^{\mathsf{T}}Ax + b^{\mathsf{T}}x + c$

Convex if A is positive semidefinite

$$E_{in}(w) = w^{\dagger}(X^{\dagger}X)w + (-2y^{\dagger}X)^{\dagger}w + y^{\dagger}y$$

 $X^{\intercal}X$ positive semidefinite?

Symmetric: Clearly

$$w^{\mathsf{T}}X^{\mathsf{T}}Xw = (Xw)^{\mathsf{T}}Xw = ||Xw||_2^2 \ge 0$$

Found Global Minimum!

- Convex = good (usually)
- Logistic Regression
 - Target function may be probaliststic
 - o Soft threshold
 - o Example: Probability of him paying loan back.
 - o Can be classifier, return most likely

Likelihood of the data. NOT $P(\theta \mid D)$

$$P(D \mid \theta) = \prod_{(x,y) \in D} p(y \mid x) = \prod_{(x,y) \in D} \underbrace{\sigma(\theta^\intercal x)^y (1 - \sigma(\theta^\intercal x))^{1-y}}_{}$$

$$\mathrm{NLL}\big(D \mid \theta\big) \, = \, - \! \sum_{x,y \in D} \! (y \ln(\sigma(\theta^\intercal x)) + (1-y) \ln(1-\sigma(\theta^\intercal x))$$

$$E_{\rm in} = \frac{1}{|D|} {
m NLL}$$

Neg. Log likelihood is convex Exercise next week (Named Cross Entropy)

??

Non-linear data

- Preprocessing / transformation of features.
- Ø og Ø^-1
- Regularization?

Learning Theory (VC Dimension, Bias Variance, Regularization and Validation)

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 - Capture the problem we consider (FBI)...
 - o 1) Ensure low Ein and 2) have Eout close to Ein
 - Hypothesis generalizes if Ein and Eout close
 - Balance between model complexity and Ein -> Eout
 - Hypothesis space / model complexity
 - Many functions can fit some data, how to find correct one
 - We want to rid the error of the dataset
- Hoeffding's Inequality?
 - o Ingen garantier, kun sandsynligheder
 - Coin flip example
 - \circ P(|v-my| > epsilon) < 2e^(-2 * epsilon^2 * N) v = sample mean, my = coin bias
 - o Overfør til classification problem. 1-0 loss. Generalization bound
 - Fixed hypothesis
 - P(|Ein Eout| > epsilon) < 2e^(-2 * epsilon^2 * N)
 - Udvidelse til P(|Ein Eout| > epsilon) < 2 M e^(-2 * epsilon^2 * N)
 - More hypothesis -> better fit -> worse generalization bound
- VC-dimension bound
 - Upper bound Eout, (propability)
 - Eout <= Ein + Omega (complexity term, VC(H))
 - Dichotomy
 - $\| \{h(x_1)...h(x_N) \text{ in } \{0,1\}^N \mid h \text{ in } H\} \| \le 2^N \|$
 - RHS længde || = skrevt $H(x_1...x_N)$
 - Growth function
 - $mH(N) = max x_1 to x_n on dichotomy$
 - Breakpoint
 - K is breakpoint if mH(N) < 2^K
 - VC(H) = max N such that mH(N) = 2^N
 - o 2D example 3 points can always be split into all dichotomies, 4 cannot

$$E_{\mathrm{out}}(g) \leq E_{\mathrm{in}}(g) + \sqrt{\frac{8}{N} \ln \frac{4m_{\mathcal{H}}(2N)}{\delta}}$$

Independent of learning algorithm, target function, input distribution

- $E_{out}(h) \le E_{in}(h) + \Omega(N, \mathcal{H}, \delta)$
- Regularization

0

- We don't want to fit the noise
- Tell the learning process to use smaller weights, unless it improves the result by a lot
- o L2
- Validation
 - o Cross-validation

Support Vector Machines (Kernels)

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$$D = \{(x, y) \mid x \in \mathbb{R}^d, y \in \{-1, 1\}\}$$

- Antag linear sceperable, many dimension makes it more likely, kernels.
- One of the best of the box
- Functional margin
 - Idea, make margin

$$\hat{\gamma}^{(i)} = y^{(i)}(w^T x + b)$$

- Correct prediction: $y_i(w^{\mathsf{T}}x_i+b)>0$
- Support vectors
- Geometrisk margin
 - o If ||w|| = 1 så er de ens
 - o Is invarient to rescaling of the parameters
 - Define same y uden hat ^

$$\gamma = \frac{\hat{\gamma}}{||w||}$$

Traning

- Max y mens vi overholder prediction
- o Dual form lets us make efficient algorithm for solving the problem we have
- Lagrange multipliers
- SVM finds the maximally separating hyperplane and is defined by "few" support vectors
- The dual optimization problem finds the support vectors (dual also convex)
- New points are classified by their weighed sum of inner products with the support vectors

Kernels

0

- Feature mapping
- $\circ \quad \mathsf{K}(\mathsf{x},\mathsf{z}) = \emptyset(\mathsf{x})^{\mathsf{h}} \mathsf{t} \, \emptyset(\mathsf{z})$
- o Fordi algo bruger kun Inner products kan vi
- Work in higher dimension space for free

$$x = (x_1, x_2), z = (z_1, z_2)$$

Polynomial kernel of degree 2

$$\begin{split} K(x,z) &= (1+x^{\mathsf{T}}z)^2 \\ &= (1+x_1z_1+x_2z_2)^2 \\ &= 1+x_1^2z_1^2+x_2^2z_2^2+2x_1z_1+2x_2z_2+2x_1z_1x_2z_2 \end{split}$$
 Feature Transform

$$(x_1, x_2) \xrightarrow{\Phi} (1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2)$$

$$\langle x, z \rangle_{\Phi} = \phi(x)^{\mathsf{T}} \phi(z)$$

$$= 1 + x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 z_1 + 2x_2 z_2 + 2x_1 z_1 x_2 z_2$$

0 Slackness

0

$$\begin{aligned} & \min_{w,b,\xi} & & \frac{1}{2}||w||^2 + C\sum_{i=1}^n \xi_i \\ & \text{S. To} & & \frac{y_i(w^\mathsf{T}x_i + b) \geq 1 - \xi_i}{\xi_i \geq 0} & \forall i \end{aligned}$$

- Little like regurlazion
- Bedre imod outliers

Neural Nets (Backpropagation, Deep Convolutional Nets)

Neuron

- Activation functions
- NN CAN approximate any continuous function (weak and useless statement in practice)
- Neural Networks are universal function approximators
- Deeper than 3 levels does not help much
- Overfitting? Add regularization and other things are better.
- Standard feed forward network
 - Layers, input

```
nn(X) = F_3(W_3F_2(W_2F_1(XW_1 + b_1) + b_2) + b_3)
```

- Non-linear, else could have been one matrix multiplication
- Weights are learned with stochastic gradient descent
- o their gradients are derived with chain rule (and computed with backpropagation).
- The derivative on each variable tells you the sensitivity of the whole expression on its value.
- Backpropagation
 - o Example
 - Not convex
 - o Gradian decent chain rule
 - Late note: preprocessing matter, affects learning rate.
 - Early stopping
- Convolutional net
 - Convolutional pooling layers -> feature detector
 - Images
 - Edge detector
- Other things
 - o recurrent networks
 - can remember, feedback
 - Good for time series, text
 - Dropout traning

Decision Trees and Ensemble Methods (Bagging, Boosting)

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 - error in and out and Error functions
 - Least squares
 - 1/0-loss
 - Capture the problem we consider (FBI)...
- Decision trees
 - Basic Construction (building blocks)
 - Good at handleing both classification and regression
 - o In base form, a white-box. Easy to interpret
 - o Can (sometimes) be plotted in 2d
- Construction
 - Many trees same function
 - Small trees should generalize better, because less rules
 - Select next attribute greedily. As in close to perfect split
 - Split that minimizes error on next level
 - Tend to overfit
 - Bias variance decomposition
- Bagging / Bootstap Aggregating (Minimize variance)
 - 1) Generate additional data from dataset
 - o 2) train
 - o 3) return majority vote or return mean prediction
 - Eout og bias variance decomposition. Bias should remain the same.
 - Any reducing in error should come from reducing variance.
 - o Random forest. Loss white-box. Knowledge of the masses
- Boosting (Mainly reduce bias)
 - Boosting Make weak learners to strong learners
 - Weak learner
 - someone that does slightly better than random
 - Small tree (2 layers maybe)
 - Have LOW variance, usually not overfitting
 - High bias because they underfit
 - Boosting: Make weak learner into strong, by combining (weak) base classifiers into powerful committee.

- Each classifier should be good at different parts of input space
- o Goal: output weighted combinations classifiers that best achieves goal

$$h(x) = \operatorname{sign}\left(\sum_{t} \alpha_{t} h_{t}(x)\right)$$

$$H(x) = \operatorname{sign}\left[0.42 + 0.21\right] + 0.92$$

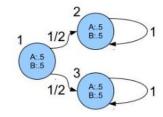
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They do better than one hypothesis both in practice and theory.

Hidden Markov Models - Decoding (Basic algorithms and applications, Viterbi and posterior decoding)

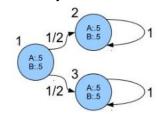
- Simpel models
 - Ovsercations are independent and identically distributed (I.I.D.)
 - Propability
 - 1st order Markov
 - Propability
- Hidden Markov model
 - o The 3 tabels. Emmission, start, and transition
 - o The joint probability
 - o Example



- o Number procision
 - Log-space
 - scaling
- Decoding (what is)
 - Finding the underlying explanation
- Viterbi decoding
 - Most likely explanation. SYNTACTICALLY correct
 - Uses w(omega) table
 - Dynamic programming
- Posterior
 - Most likely state to be in in the n'th step
 - Alpha (forward algo) og beta (backward algo)

Hidden Markov Models - Training (Basic algorithms and applications, building models and selecting initial model parameters)

- Simpel models
 - Ovsercations are independent and identically distributed (I.I.D.)
 - Propability
 - 1st order Markov
 - Propability
- Hidden Markov model
 - o The 3 tabels. Emmission, start, and transition
 - The joint probability



- Example
- o Number procision
 - Log-space
 - Scaling
- Building a model
 - Talk about DNA handin
 - Domain knowledge
 - We can define sequences, setting all output to 1
- Training
 - Counting and Psudo-counting
 - We have a lot of X (observations) and Z
 - Intuition: Parameters should reflect what we have seen
 - Emission and transition
- Viterbi training
 - Viterbi decoding = Most likely explanation. SYNTACTICALLY correct
 - Finds local maximum of p(X,Z|HMM)
 - 1. Decide on some initial parameter θ°
 - Find the most likely sequence of states Z* explaining X using the the Viterbi Algorithm and the current parameters θ¹
 - 3. Update parameters to θⁱ⁺¹ by "counting" (with pseudo counts) according to (**X**,**Z***).
 - Repeat 2-3 until P(X,Z* | θ') is satisfactory (or the Viterbi sequence of states does not change).

Unsupervised Learning - Clustering

- General clustering
 - Group set of data
 - Unsupervised (no labels)
 - Trying all partitions to minimize some function is too expensive
 - Example, what is a good cluster and a bad one.
- K-means clustering
 - o Partitioning algorithm, find k partitions and minimize function.
 - Imprice iteratively

$$\mu_C = \frac{1}{|C|} \sum_{x_i \in C} x_i$$

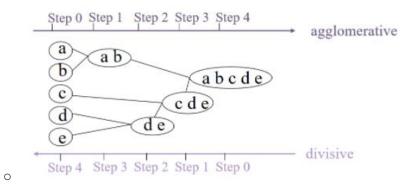
Centroid of a cluster

$$TD(C_j) = \sqrt{\sum_{p \in C_j} dist(p, \mu_{C_j})^2}$$

- Cluster compactness measure
- Clustering compactness measure (ideal clustering minimizes this)

$$TD = \sqrt{\sum_{j=1}^{k} TD^2(C_j)}$$

- Lloyd's algorithm
 - + Relatively efficient
 - Specify k
- Clusters forced to have convex shape
- Result and runtime dependent on initial partition
- Often tends at local optimum
- K-medoid
 - Better against noise
 - Works in spaces where mean not defined, L1 norm (manhatten dis)
 - Selecting k: Silhouette coefficient. Increasing k will always make TD better
- Density-based clustering
 - Cluster are dense regions separated by non-dense regions
 - Example: Snake example?
 - o Outliers
 - Core objects. MinPts and epsilon needs to be learned
 - o Epsilon: Graph and take first valley minPts have heuristic math formel.
- Hierarchical clustering
 - Clustering at different level
 - Single-link (min), complete (max), avg



Unsupervised Learning - Outlier Detection and Dimensionality Reduction

- Outlier
 - A things that's so different that it might be an error
 - Meaning
 - Might be fraud
 - Surveillance
 - Data cleaning
 - Be careful of removing outliers, might be valid data and if you don't notice you might learn something incorrect.
- Unsupervised outlier detection
 - Similar to clustering
 - Perspektiver til Density-based clustering
 - Every object not in a cluster is an outlier
 - Distance based
 - DB(precentage, distance)
 - Global based
- Local outlier
 - Compare distance to neighbors based on own distance
 - Note angle in high dimension
- Dimensionality reduction
 - Why: Reduce data, but keep structure/information. Make the data cheaper/better/easier to handle.
 - Project data to lower space.
 - We want to keep variance
 - Number billeder. PCA (principal components) 784 dim -> 49 dim
 - Preprocessing: scale and zero mean