# CS489: Machine Learning

Michael Noukhovitch

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# 1 Introduction

machine learning giving computers ability to learn without being explicitly programmed

A machine learns from experience E wrt to some class of tasks T and performance measure P if its performance in task T, as measured by P, improves with E

#### Three types:

- supervised
- unsupervised
- reinforcement

#### Long-term goals:

- meta-programming
- lifelong machine learning
- transfer learning

# 1.1 Supervised Learning

**Definition.** given a training set of examples (x, f(x)), return a hypothesis h that approximates h

Two types:

classification where output space consists of categorical values

**regression** where output space consists of numerical values

#### 1.1.1 Hypothesis Space

hypothesis space set of all hypotheses H that the learner may consider

**consistent** if hypothesis h agrees with f on all examples

realizable if the hypothesis space constains the consistent function

our objective can be restated as a search problem to find the hypothesis h in hypothesis space H that minimizes some objective

# 2 Nearest Neighbour

#### 2.1 Basic NN

nearest neighbours label any example with the label of its nearest neighbours

```
classification: h(x) = y_{x*} where y_{x*} = \operatorname{argmin}_{x'} d(x, x') is the label associated with the nearest neighbour
```

#### 2.2 KNN

**k-nearest neighbours** assign the most frequent label among k nearest neighbours

let knn(x) be the k nearest neighbours then  $y_x = \text{mode}(y_{x'}|x' \in knn(x))$ 

**overfitting** a hypothesis h with training accuracy higher than its own testing accuracy  $\max(0, \operatorname{trainAccuracy}(h) - \operatorname{testAccuracy}(h))$ 

- classifier too expressive
- noisy data
- lack of data

**underfitting** a hypothesis h with training accuracy lower than testing accuracy of some other hypothesis h',  $\max(0, \max_{h'} \operatorname{trainAccuracy}(h) - \operatorname{testAccuracy}(h'))$ 

• classifier not expressive enough

k-fold cross validation split data in k equal subsets, run k experiments testing on one subset, and training on all the others. Report average accuracy

weighted knn weight each neighbour by distance

**knn regression**  $y_x$  is a real value,  $y_x \leftarrow average(y_{x'}|x' \in knn(x))$ 

properties:

- + lazy learning (learn on test)
- + conceptually simple
- + flexible decision boundaries
- good distance measures are hard to find
- noise can strongly influence
- can't handle more than a few dozen attributes/features
- requires a lot of computation and memory

# 3 Linear Regression

#### 3.1 Least Squares

find linear hypothesis h:  $t = w^T \bar{x}$ , find w to minimize euclidean L2 loss

$$w* = argmin_w \frac{1}{2} \sum_{n=1}^{N} (t_n - w^T \bar{x}_n)^2$$

where  $\bar{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$  and we can solve with  $w = A^{-1}b$  or Aw = b which can be solved as a linear system

#### 3.1.1 Regularization

Least squares can be unstable, overfit, so change optimization

$$w* = argmin_{w} \frac{1}{2} \sum_{n=1}^{N} (t_{n} - w^{T} \bar{x}_{n})^{2} + \frac{\lambda}{2} \|w\|_{2}^{2}$$

or 
$$(\lambda I + A)w = b$$

#### 3.2 Maximum Likelihood

derive the same thing but from a different perspective: assume  $y = w^T \bar{x} + \text{gaussian noise so}$ 

$$Pr(y|\bar{X}, w, \sigma) = N(y|w^T\bar{X}, \sigma^2)$$

$$w* = argmax_w Pr(y|\bar{X}, w, \sigma)$$
...
$$= argmin_w \sum_n (y_n - w^T\bar{x}_n)^2$$

which is the same as least squares

#### 3.3 Maximum A Posteriori

find w\* with highest posterior probability, knowing that prior  $P(w) = N(0, \Sigma)$ 

$$Pr(w|X,y) \propto Pr(w)Pr(y|X,w)$$

therefore for optimization:

$$w* = argmax_w Pr(w|\bar{X}, y)$$
...
$$= argmin_w \sum_n (y_n - w^T \bar{x}_n)^2 + w^T \Sigma^{-1} w$$

let  $\Sigma^{-1} = \lambda I$ 

$$= argmin_w \sum_{n} (y_n - w^T \bar{x}_n)^2 + \lambda \|w\|_2^2$$

and we arrive at least squares with regularization

#### 3.4 Expected Squared Loss

$$E[loss] = \int_{x,y} Pr(x,y)(y - w^T \bar{x})^2 dx dy$$

$$= \int_{x,y} Pr(x,y)(y - f(x))^2 + \int_x Pr(x)(f(x) - w^T \bar{x})^2 dx$$

$$= \text{noise (constant)} + \text{error (relative to } w)$$

lets consider the expected error wrt our dataset S

$$E[error] = E_S[(f(x) - w_S^T)^2]$$

$$= (f(x) - E_S[w_S^T \bar{x}])^2 + E_S[(E_S[w_S^T \bar{x}] - w_S^T \bar{x})^2]$$

$$= \text{bias}^2 + \text{variance}$$

therefore putting it together

$$E[loss] = bias^2 + variance + noise$$

# 3.5 Bayesian Linear Regression

instead of using w\*, compute weighted avg prediction using  $Pr(w|\bar{X},y)$ 

$$Pr(w|\bar{X}, y) = N(\bar{w}, A^{-1})$$

where 
$$w = \sigma^{-2}A^{-1}\bar{X}^Ty$$
 
$$A = \sigma^{-2}\bar{X}^T\bar{X} + \Sigma^{-1}$$

# 3.6 Bayesian Prediction

let  $x_*$  be the input for which we predict  $y_*$ 

$$Pr(y_*|\bar{x}_*, \bar{X}, y) = \int_w Pr(y_*|\bar{x}_*, w) Pr(w|\bar{X}, y) dw$$
...
$$= N(\bar{x}_*^T A^{-1} \bar{X}^T y, \bar{x}_*^T A^{-1} \bar{x}_*)$$

# 4 Statistical Learning

#### 4.1 Introduction

**probability distribution** a specific probability for each event in our sample space **joint distribution** spec of probabilities for all combinations of events  $Pr(A \wedge B)$  conditional probabilities  $Pr(A|B) = Pr(A \wedge B)/Pr(B)$ 

# 4.2 Bayes Rules

$$Pr(B|A) = \frac{Pr(A|B)Pr(B)}{Pr(A)}$$

posterior P(B|A)

likelihood P(A|B)

prior P(B)

normalizing P(A)

evidence A

# 4.3 Bayesian Learning

computing the posterior of hypothesis given evidence using Bayes' theorem:

$$Pr(H|e) = kPr(e|H)Pr(H)$$

where k is a normalization constant such that the sum of all Pr(H|e) = 1 properties:

- + optimal (given prior)
- + no overfitting (all hypotheses considered)
- intractable if hypothesis space is large

prediction:

$$Pr(X|e) = \sum_{i} Pr(X|h_i)P(h_i|e)$$

# 4.4 Approximate Bayesian Learning

Maximum A Posteriori make prediction based on most probable hypothesis (vs basing on all hypotheses weighted by probability)

$$h_{map} = argmax_{h_i}Pr(h_i|e)$$

$$= argmax_{h_i}Pr(e|h_i)Pr(h)$$

$$Pr(X|e) = Pr(X|h_{map})$$

- + controlled overfitting
- + converges as data increases
- less accurate than Bayesian prediction
- maybe be intractable!

**Maximum Likelihood** simplify MAP by assuming uniform prior  $Pr(h_i) = Pr(h_j) \forall i, j$ 

$$h_{ml} = argmax_{h_i} Pr(e|h_i)$$
$$Pr(X|e) = Pr(X|h_{ml})$$

- + still converges
- least accurate because ignore prior info
- overfits

also, can be easier than MAP:  $h_{ml} = argmax_h \sum_n \log Pr(e_n|h)$ 

# 5 Mixture of Gaussians

#### 5.1 Introduction

Assume:

- each prior is frequency:  $Pr(C = c_k) = \pi_k$
- Pr(x|C) is gaussian
- covariance matrix  $\Sigma$  is used for each class

We can use maximum likelihood to estimate the parameters:

$$Pr(x|c_k) \propto e^{-\frac{1}{2}(x-\mu_k)^T \Sigma^{-1}(x-\mu_k)}$$

Where:

$$\pi = \frac{\sum_{n} y_{n}}{N}$$
 average  $y$ 

$$\mu_{k} = \frac{\sum_{n \in c_{k}} x_{n}}{N_{k}}$$
 mean of class  $k$ 

$$\Sigma = \frac{N_{1}}{N} S_{1} + \frac{N_{2}}{N} S_{2} \dots$$
 covariance
$$S_{k} = \frac{1}{N_{k}} \sum_{n \in c_{k}} (x_{n} - \mu_{k})(x_{n} - \mu_{k})^{T}$$
 weighted variance

#### 5.2 Two Class

Then if there are two classes  $c_k$  and  $c_j$ ,

$$Pr(c_k|x) = \frac{1}{1 + e^{-(w^T x + w_0)}}$$
$$= \sigma(w^T x + w_0)$$

where 
$$w = \Sigma^{-1}(\mu_k - \mu_j)$$
  

$$w_0 = -\frac{1}{2}\mu_k^T \Sigma^{-1} \mu_k + \frac{1}{2}\mu_j^T \Sigma^{-1} \mu_j + \ln \frac{\pi_k}{\pi_j}$$

choose the best class as the one with probability > 0.5, so class boundary is at

$$\sigma(w_k^Tx + w_0) = 0.5$$
 
$$w_k^T\bar{x} = 0 \text{ is a linear separator}$$

#### 5.3 Multi-class

Normalize using softmax:

$$Pr(c_k|x) = \frac{Pr(c_k)Pr(x|c_k)}{\sum_j Pr(c_j)Pr(x|c_j)}$$
$$= \frac{e^{w_k^T \bar{x}}}{\sum_j e^{w_j^T \bar{x}}}$$

# 6 Logistic Regression

### 6.1 Introduction

MoG is restrictive, assumes everything is a gaussian. Generalize to exponential family:

$$Pr(x|\Theta_k) = \exp(\Theta_k^T T(x) - A(\Theta_k) + B(x))$$

where  $\Theta_k$ : parameters of class k

 $T(x), A(\Theta_k), B(x)$ : arbitrary functions

and the posterior  $Pr(c_k|x) = \sigma(w^T x + w_0)$  which we will learn directly by maximum likelihood, in general it is

- logistic sigmoid for binary
- softmax for multiclass

#### 6.2 Logisite Regression Classification

For some dataset (X, y) and for two classes  $y \in 0, 1$ :

$$w^* = argmax_w \prod_n \sigma(w^T \bar{x}_n)^{y_n} (1 - \sigma(w^T \bar{x}_n))^{1-y_n}$$

so our objective is

$$L(w) = -\sum_{n} y_n \ln \sigma(w^T \bar{x}_n) + (1 - y_n) \ln(1 - \sigma(w^T \bar{x}_n))$$

finding the min by setting derivative to 0

$$\frac{dL}{dw} = 0$$

$$0 = \sum_{n} [\sigma(w^T \bar{x}_n) - y_n] \bar{x}_n$$

and since we can't isolate w we use **Newton's Method** to iteratively solve:

$$w \to w - H^{-1} \nabla L(w)$$

where  $H = \bar{X}R\bar{X}^T$  is the hessian

$$R = \begin{bmatrix} \sigma_1(1 - \sigma_1) & & \\ & \dots & \\ & & \sigma_N(1 - \sigma_N) \end{bmatrix}$$
$$\sigma_k = \sigma(w^T \bar{x}_k)$$

# 6.3 Regularization

To ensure that we can inverse H (so it isn't singular), add  $\lambda$ :

$$H = \bar{X}R\bar{X}^T + \lambda I$$

# 6.4 Non-linear Regression

Non-linear regression using the same algorithm, map inputs to a different space! Use non-linear basis functions  $\phi_i$ , so for

$$\phi_0(x) = 1$$

$$\phi_1(x) = x$$

$$\phi_2(x) = x^2$$

the hypothesis space is  $H = \{x \leftarrow w_0\phi_0(x) + w_1\phi_1(x) + w_2\phi_2(x) | w_i \in \Re\}$ 

common basis functions:

- polynomial  $\phi_i(x) = x^j$
- gaussian  $\phi_j(x) = e^{-\frac{(x-\mu_j)^2}{2s^2}}$
- sigmoid  $\phi_j(x) = \sigma(\frac{x-\mu_j}{s})$
- fourier, wavelets ...

# 7 Perceptron

## 7.1 Computer vs Brain

Computer:

- bunch of gates
- electrical signals by gates
- sequential and parallel
- fragile

Brain

• network of neurons

- nerve signal propogate
- parallel
- robust (neurons die)

ANN Unit consists of weights w and activation function h, so that output  $y_j = h(W_j \bar{x})$ . Structure is either **feed-forward** or **recurrent** 

# 7.2 Perceptron Learning

```
Learning is done separately for each unit j:

for all pairs (x,y) do

if output is correct then

Do nothing

else if output = 0, label = 1 then

\forall_i W_{ji} \to W_{ji} + x_i

else if output = 1, label = 0 then

\forall_i W_{ji} \to W_{ji} - x_i

end if

end for
```

# 7.3 Alternative Learning

let M be the set of misclassified examples (where  $y_n w^T \bar{x}_n < 0$ ) then find w to minimize number of misclassifications:

$$E(w) = -\sum_{(x_n, y_n) \in M} y_n w^T \bar{x}_n$$

Use gradient descent

$$w \leftarrow w - \eta \nabla E$$

where  $\eta$  is the learning rate

If we adjust w one example at a time, we use **sequential gradient descent** which is equivalent to threshold perceptron learning when  $\eta = 1$ 

#### 7.4 Linear Separability

Threshold perceptron converges iff the data is linearly separable

linear separator  $w^T \bar{x}$ , since it is linear in w

#### 7.5 Other Networks

Sigmoid Perceptron "soft" linear separators (same H as linear regression)

$$E(w) = \frac{1}{2} \sum_{n} (y_n - \sigma(w^T \bar{x}_n))^2$$

for all 
$$(x_n, y_n)$$
 do
$$E_n \leftarrow y_n - \sigma(w^T \bar{x}_n)$$

$$w \leftarrow w + \eta E_n \sigma(w^T \bar{x}_n) (1 - \sigma(w^T \bar{x}_n)) \bar{x}_n$$
end for

# 8 Multilayer Neural Networks

#### 8.1 Introduction

Previously, our basis functions were fixed, but we can remove that restriction by learning non-linear basis functions.

hidden unit 
$$z_j = h_1(w_j^{(1)}\bar{x})$$
  
output unit  $y_k = h_1(w_j^{(2)}\bar{x})$   
both units  $y_k = h_2(\sum_j w_{kj}^{(2)} h_1(\sum_i w_{ji}^{(1)} x_i))$ 

if we consider our hidden input to be a basis function, then this is equivalent to a linear regression and a learned basis function, e.g.

- non-linear regression:  $h_1$  is a non-linear function,  $h_2$  is identity
- $\bullet$  non-linear classification:  $h_1$  is a non-linear function,  $h_2$  is sigmoid

# 8.2 Backpropogation

Error function:

$$E(w) = \frac{1}{2} \sum_{n} \|f(x_n, W) - y_n\|_2^2$$
 where  $f(x, W) = \sum_{i} w_{kj}^{(2)} \sigma(\sum_{i} w_{ji}^{(1)} x_i)$ 

so our update rule for gradient descent is

$$w_{ji} \leftarrow w_{ji} - \eta \frac{\delta E_n}{\delta w_{ji}}$$
 where  $\frac{\delta E_n}{\delta w_{ji}} = \delta_j z_i$ 

Do gradient update in two phases:

1. **forward**: compute output  $z_i$  of each unit j

$$z_j = h(\sum_i w_{ji} z_i)$$

2. backward: compute delta  $\delta_i$  at each unit j

$$d_j = \begin{cases} h'(a_j)(z_i - y_i), & \text{if } j \text{ is output} \\ h'(a_j) \sum_k w_{kj} \delta_k & \text{if } j \text{ is a hidden unit before } k \end{cases}$$

Analysis:

- fast computation
- slow convergence, may get trapped in local optima
- prone to overfitting, solve with
  - early stopping
  - regularization

## 9 Kernel Methods

#### 9.1 Introduction

Data may not be linearly separable, so map into a high-dimensional space where it is! This is computationally difficult though, so instead calculate a similarity measure (dot product) in the high dimensional space and use algorithms that only need that measure.

**kernel methods** use large set of fixed non-linear basis functions, with a "dual trick" to make complexity depend on amount of data instead of number of basis functions

**kernel function**  $k(x, x') = \phi(x)^T \phi(x')$  for some basis function  $\phi(x)$ 

linear regression objective, setting derivative to 0 gives us

$$w = -\frac{1}{\lambda} \sum_{n} (w^{T} \phi(x_n) - y_n) \phi(x_n)$$

so w is a linear combination of inputs in feature space

$$= \{\phi(x_n) | 1 \le n \le N\}$$
substitute  $w = \phi a$ 
where  $\phi = [\phi(x_1) \dots \phi(x_n)]$ 

$$a = [a_1, \dots a_n]^T$$

now let  $K = \Phi^T \Phi$ , therefore our prediction

$$y_* = \phi(x_*)^T \Phi a$$
  
=  $k(x_*, X)(K + \lambda I)^{-1}y$ 

For this we need to just find dual solution a instead of w

- now depends on # of data instead of # of basis function
- can use many more basis functions
- don't actually need  $\Phi$ , just need a semi-definite kernel  $K, \exists \Phi \mid K = \Phi^T \Phi$  or all eigenvalues  $\geq 0$

#### 9.2 Common Kernels

Common kernels:

- polynomial  $k(x, x') = (x^T x' + c)^M, c \ge 0$
- gaussian  $k(x, x') = \exp(-\frac{\|x x'\|^2}{2\sigma^2})$

Also construct more kernels using rules. Let  $k_1(x, x')$  and  $k_2(x, x')$  be valid kernels, and  $x = \begin{pmatrix} x_a \\ x_b \end{pmatrix}$  then it is also valid k(x, x') =

- $ck_1(x, x') \forall c > 0$
- $f(x)k_1(x,x')f(x') \forall f$
- $q(k_1(x,x'))$  where q is a polynomial with coeffs  $\geq 0$
- $\exp k_1(x,x')f(x')$
- $k_1(x,x') + k_2(x,x')$
- $k_1(x,x')k_2(x,x')$
- $k_3(\phi(x),\phi(x'))$
- $x^T A x'$  where A is symmetric positive semi-definite
- $k_a(x_a, x'_a) + k_b(x_b, x'_b)$
- $k_a(x_a, x'_a)k_b(x_b, x'_b)$

Kernels can also be defined wrt to sets, strings, graphs. E.g.  $k(d_1, d_2) = \text{similarity between}$  two documents

#### 9.3 Example

Show that  $k(x,z)=(x^Tz)^2$  is a valid kernel by finding  $\phi$ 

$$k(x,z) = (x^T z)^2$$

$$= (x_1 z_1 + x_2 z_2)^2$$

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

$$= (x_1^2, \sqrt{2}x_1 x_2, x_2^2)(z_1^2, \sqrt{2}z_1 x_2, z_2^2)^T$$

$$= \phi(x)^T \phi(z)$$

after separating x and z we find that

$$\phi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)^T$$

## 10 Gaussian Processes

#### 10.1 Overview

We want to do regression even when we don't know the exact type of function. We assume that p(f(x)) is a gaussian for all points x, and use a kernel function as the distance between any two points. Then we can find a general function f

$$f(x) = GP(\text{mean, kernel covariance})$$
  

$$m(x) = E(f(x))$$
  

$$k(x, x') = E((f(x) - m(x))(f(x') - m(x')))$$

# 10.2 Gaussian Process Regression

$$\begin{aligned} & \text{prior } p(f(x)) & = N(m(x), k(x, x)) \\ & \text{likelihood } p(y|X, f) & = N(f(x), \sigma^2 I) \\ & \text{posterior } p(f(x)|X, y) = N(\bar{f}(x), k'(x, x)) \\ & \text{where } \bar{f}(x) & = k(x, X)(K + \sigma^2 I)^{-1} y \\ & \quad k'(x, x) & = k(x, x) - k(x, X)(K + \sigma^2 I)^{-1} k(X, x) \\ & \text{prediction } p(y|x, X, y) & = N(\bar{f}(x), k'(x, x)) \end{aligned}$$

Inversion of  $K + \sigma I$  (and therefore this process) is cubic in number of training points (vs bayesian linear regression which is cubic in number of basis functions

# 11 Support Vector Machines

#### 11.1 Overview

Find a separator such that it has maximum margins with nearest data

$$\max_{x} \frac{1}{\|w\|} (\min_{n} y_n w^T \phi(x_n))$$

Fix the minimal distance to 1, minimize ||w||

$$\min_{w} \frac{1}{2} \|w\|^2$$
s.t.  $y_n w^T \phi(x_n) \ge 1 \,\forall n$ 

The points that decide our separator, where  $y_n w^T \phi(x_n) = 1$ , are known as the **support** vectors

#### 11.2 Dual

Reformulate as penalty for  $x_n$  violating constraint

$$\max_{a>0} \min_{w} L(w, a)$$
 where  $L(w, a) = \frac{1}{2} \|w\|^2 - \sum_{n} a_n (y_n w^T \phi(x_n) - 1)$ 

substitute  $w = \sum_{n} a_n y_n \phi(x_n)$ 

$$\max_{a} L(a)$$
 s.t.  $a_n \ge 0$ 

where 
$$L(a) = \sum_{n} a_n - \frac{1}{2} \sum_{n} \sum_{n'} a_n a_{n'} y_n y_{n'} k(x_n, x_{n'})$$

It can be sparse (many  $a_n$ s are 0) and also classification only needs the kernel

$$y_* = sign(\sum_n a_n y_n k(x_n, x_*))$$

### 11.3 Comparison to Perceptron

Perceptron:

- linear separator
- simple update rule
- prone to overfitting

SVM:

- unique max-margin linear separator
- quadratic optimization
- robust to overfitting

#### 11.4 Soft Margins

If the data is not linearly separable, relax constraints to allow for misclassification:

$$y_n w^T \phi(x_n) \ge 1 - \epsilon_n, \epsilon_n \ge 0 \quad \forall n$$

Objective is to minimize the misclassification (as denoted by  $\epsilon$ )

$$\min_{w,\epsilon} C \sum_{n=1}^{N} \epsilon_n + \frac{1}{2} \left\| w \right\|^2$$

- $\bullet$   $\,C$  acts as the tradeoff between error minimization and model complexity
- $C \to \infty$  gives the hard margin
- can handle minor misclassifications but still sensitive to outliers
- all points on the margin, inside the margin, or misclassified are support vectors

#### 11.5 Mulitclass SVM

#### 11.5.1 One-against-all

Train k SVMs to distinguish each class from the rest, but two classes might both say the example belongs to them

#### 11.5.2 Pairwise Comparison

Train  $O(k^2)$  SVMs to compare between each pair of classes

#### 11.5.3 Continuous Ranking

Single SVM that returns a continuous value to rank all classes

$$y_* = argmax_k w_k^T \phi(x_*)$$

Multi-class margin:

for each class  $k \neq y$  define a linear constant

$$w_y^T \phi(x) - w_k^T \phi(x) \ge 1$$

therefore the optimization is

$$\min_{w} \frac{1}{2} \sum_{k} \|w_k\|^2$$
  
s.t.  $w_{y_n}^T \phi(x_n) - w_k^T \phi(x_n) \ge 1 \ \forall n, k \ne y_n$ 

## 12 Hidden Markov Model

#### 12.1 Assumptions

1. stationary process: transition and emission is the same at each step

$$Pr(x_t|y_t) = Pr(x_{t+1}|y_{t+1}) \ \forall t$$
$$Pr(y_t|y_{t-1}) = Pr(y_{t+1}|y_t) \ \forall t$$

2. markovian process: next state only depends on previous

$$Pr(y_{t+1}|y_t, y_{t-1}...y_1) = Pr(y_{t+1}|y_t) \ \forall t$$

#### 12.2 Inference

- monitoring  $Pr(y_t|x_{1...t})$
- prediction  $Pr(y_{t+k}|x_{1...t})$
- hindsight  $Pr(y_k|x_{1...t})$  where k < t
- most likely estimation  $argmax_{y_1...y_t} Pr(y_{1...t}|x_{1...t})$

#### 12.2.1 Monitoring

$$P(y_t|x_{1...t}) = Pr(x_t|y_t) \sum_{y_{t-1}} Pr(y_t|y_{t-1}) Pr(y_{t-1}|x_{1...t-1})$$

1. Compute  $Pr(y_t|x_{1...t})$  with forward algorithm:

$$\begin{array}{l} Pr(y_{1}|x_{1}) \propto Pr(x_{1}|y_{1})Pr(y_{1}) \\ \textbf{for } i = 1 \rightarrow k \ \textbf{do} \\ Pr(y_{i}|x_{1...i}) \propto Pr(x_{i}|y_{i}) \sum_{y_{i-1}} Pr(y_{i}|y_{i-1})Pr(y_{i-1}|x_{1...i-1}) \\ \textbf{end for} \end{array}$$

#### 12.2.2 Prediction

$$Pr(y_{t+k}|x_{1...t}) = \sum_{y_{t+k-1}} Pr(y_{t+k}|y_{t+k-1}) Pr(y_{t+k-1}|x_{1...t})$$

- 1. Compute  $Pr(y_t|x_{1...t})$  with forward algorithm as previously
- 2. Compute  $Pr(y_{t+k}|x_{1...t})$  with forward algorithm:

for 
$$i = 1 \to k$$
 do  $Pr(y_{t+i}|x_{1...t}) = \sum_{y_{i-1}} Pr(y_{t+i}|y_{t+i-1}) Pr(y_{t+i-1}|x_{1...t})$  end for

#### 12.2.3 Hindsight

$$Pr(y_k|x_{1...t}) = Pr(y_k|x_{1...k})Pr(x_{k+1...t}|y_k)$$

- 1. Compute  $Pr(y_t|x_{1...t})$  with forward algorithm as previously
- 2. Compute  $Pr(x_{k+1...t}|y_k)$  with backwards algorithm:

for 
$$i=t-1 \rightarrow k$$
 do 
$$Pr(x_{i...t}|y_{i-1}) = \sum_{y_i} Pr(y_i|y_{i-1}) Pr(x_i|y_i) Pr(x_{i+1...t}|y_i)$$
 and for

3. Compute  $Pr(y_k|x_{k+1...t}) = Pr(x_{k+1...t}|y_k)$ 

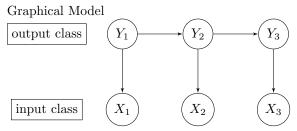
#### 12.2.4 Most Likely Explanantion

Most likely sequence of events (classes) given measuresments

$$\underset{y_{1...t}}{argmax_{y_{1...t}}} Pr(y_{1...t}|x_{1...t}) \\ \max_{y_{1...t}} Pr(y_{1...t}|x_{1...t}) = \max_{y_{t}} Pr(x_{t}|y_{t}) \max_{y_{1...t-1}} Pr(y_{1...t}|x_{1...t-1})$$

Compute  $\max_{y_1...t} Pr(y_{1...t}|x_{1...t})$  with dynamic programming, **Viterbi Algorithm**  $Pr(y_{1...2}|x_1) \propto \max_{y_1} Pr(y_2|y_1) Pr(x_1|y_1) Pr(y_1)$  for  $i = 2 \to t - 1$  do  $Pr(y_{1...i+1}|x_{1...i}) \propto \max_{y_i} Pr(y_{i+1}|y_i) Pr(x_i|y_i) \max_{y_{1...i-1}} Pr(y_{1...i}|x_{1...i-1})$  end for  $Pr(y_{1...t}|x_{1...t}) \propto \max_{y_t} Pr(x_t|y_t) \max_{y_{1...t-1}} Pr(y_{1...t}|x_{1...t-1})$ 

#### 12.3 Parametrization



Parametrized distributions:

- transition  $P(Y_t|Y_{t-1}) = Mulitnomial_{Y_{t-1}}$
- emission  $P(X_t|Y_t) = Gaussian(\mu_y, \sigma_y)$
- start  $P(Y_1) = Multinomial$
- joint  $P(X_{1:k}, Y_{1:k}) = P(Y_1) \prod_{t=1}^k P(X_t | Y_t) \prod_{t>1}^k P(y_t | y_{t-1})$

# 12.4 Supervised Learning

#### 12.4.1 Multinomial Emissions

Objective:

$$argmax_{\pi,\theta,\phi} Pr(y_{1...t}, x_{1...t} | \pi, \theta, \phi)$$

For  $y \in \{c_1, c_2\}, x \in \{v_1, v_2\}$ , maximum likelihood:

$$\begin{split} &\pi_{c_1^{\text{start}}} = \#c_1^{\text{start}}/(c_1^{\text{start}} + c_2^{\text{start}}) \\ &\theta_{c1|c1} = \#(c_1, c_1)/(\#(c_1, c_1) + \#(c_2, c_1)) \\ &\theta_{c1|c2} = \#(c_1, c_2)/(\#(c_1, c_2) + \#(c_2, c_2)) \\ &\phi_{v1|c1} = \#(v_1, c_1)/(\#(v_1, c_1) + \#(v_2, c_1)) \\ &\phi_{v1|c2} = \#(v_1, c_2)/(\#(v_1, c_2) + \#(v_2, c_2)) \end{split}$$

#### 12.4.2 Gaussian Emissions

$$\pi_{c_1^{\text{start}}} = \#c_1^{\text{start}}/(c_1^{\text{start}} + c_2^{\text{start}})$$

$$\theta_{c1|c1} = \#(c_1, c_1)/(\#(c_1, c_1) + \#(c_2, c_1))$$

$$\theta_{c1|c2} = \#(c_1, c_2)/(\#(c_1, c_2) + \#(c_2, c_2))$$

$$\mu_{c1} = \text{mean of } c_1$$

$$\mu_{c2} = \text{mean of } c_2$$

$$\sigma_{c1}^2 = \frac{1}{\#c_1} \sum_{t|y_t = c_1} (x_t - \mu_{c_1})^2$$

$$\sigma_{c2}^2 = \frac{1}{\#c_2} \sum_{t|y_t = c_2} (x_t - \mu_{c_2})^2$$

#### 12.4.3 Monitoring and MLE

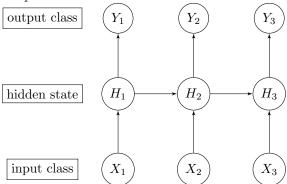
**Monitoring**: what is the probability of  $y_i = c_1$  at any i? iterate  $Pr(y_i|x_{1...i}) \propto Pr(x_i|y_i) \sum_{y_{i-1}} Pr(y_i|y_{i-1}) Pr(y_{i-1}|x_{1...i-1})$ 

Most Likely Explanation:  $argmax_{y_1...y_t}Pr(y_{1...t}|x_{1...t})$ ? Viterbi algorithm! iterate  $\max_{y_{1...i}} Pr(y_{1...i+1}|x_{1...i}) \propto \max_{y_i} Pr(y_{i+1}|y_i)Pr(x_i|y_i) \max_{y_{1...i-1}} Pr(y_{1...i}|x_{1...i-1})$ 

Example 12.1. Belief Monitoring and Most Likely Sequence see CS489-HMM.pdf

# 13 Recurrent Neural Networks

Graphical Model:



HMMs have more flexible queries, RNNs have more expressive distributions

## 13.1 Belief Monitoring

 $P(Y_1, X_1) =$ 

- sigmoid or softmax (distribution over binary and categorial outputs)
- linear (gaussian distribution with unit variance)

# 14 Deep Neural Networks

#### 14.1 Overview

Deep Neural Network ann with many hidden layers

- + high expressiveness
- vanishing gradient
- avoiding overfitting

Applications:

- speech recognition
- image recognition: ImageNet (3.07% by Inception V4)

- machine translation
- control ...

# 14.2 Vanishing Gradient

With sigmoid and hyperbolic activation function, gradient is always leq 1. Therefore, since backprop at each layers multiplies by gradient, the gradient becomes very small as we progress back through layers

$$\frac{\delta y}{\delta w_4} = \sigma'(a_4)\sigma(a_3)$$

$$\frac{\delta y}{\delta w_3} = \sigma'(a_4)w_4\sigma'(a_3)\sigma(a_2) \le \frac{\delta y}{\delta w_4}$$

Solutions:

- pre-training
- ReLU  $h(a) = \max(0, a)$ 
  - gradient is 0 or 1
  - sparse computation
  - softplus  $h(a) = \log(1 + e^a)$
- Maxout: learn a piecewise activation function that is the max of k linear functions (used with dropout)
  - $-h_i(x) = \max_{j \in [1,k]}(z_{ij}) \text{ where } z_{ij} = x^T W_{...ij} + b_{ij}$
  - doesn't have any places where gradient is close to 0
  - enhances accuracy of dropout averaging

# 14.3 Overfitting

High expressivity increases risk of overfitting Solutions:

- regularization
- data augmentation
- dropout: randomly drop some units from the network when training
  - training: unit x is dropped with prob p
  - testing: multiply output of unit x by 1-p
  - approximate form of ensemble learning

# 15 Convolutional Neural Networks

#### 15.1 Convolutions

continuous

$$y(i) = \int_{t} x(t)w(i-t)dt$$
$$= (x * w)(t)$$

discrete

$$y(i) = \sum_{-\infty}^{\infty} x(t)w(i-t)dt$$

Example 15.1. vertical edge detection

$$y(i,j) = x(i,j) - x(i-1,j)$$

$$w(i-t_1, j-t_2) = \begin{cases} 1, & \text{if } t_1 = i, t_2 = j \\ -1, & \text{if } t_1 = i+1, t_2 = j \\ 1, & \text{otherwise} \end{cases}$$

# 15.2 CNN

In neural networks

**convolution** linear combination of a subset of units based on a specific pattern of weights **pooling** commutative math operation combining several units (max, min, average ...)

**CNN** network with alternating convolution and pooling, where some convolution weights are shared

$$a_j = \sum_i w_{ji} z_i$$

combine with an activation function to produce a feature

$$z_j = h(\sum_i w_{ji} z_i)$$

Benefits:

- sparse interactions
- parameter sharing
- locally equivarient

- locally invariant to translation
- handle inputs of varying length

#### Applications:

- image processing
- data with sequential, spatial, or tensor patterns

# 16 Recurrent and Recursive Neural Networks

#### 16.1 Recurrent Neural Network

Output is fed back to the network as inputs, so the network can unroll to handle variable length data

- train with BPTT, by unrolling the network a number of steps
- weight sharing combines gradients of shared weights into single gradient
- $\bullet$  challenges
  - gradient vanishing and exploding
  - long range memory
  - prediction drift

Long Short Term Memory (LSTM) networks tackle that challenge by using gates to control memory (input, forget, output)

#### 16.1.1 Uses

- belief monitoring
  - RNN can simulate and generalize HMM
- bi-directional RNN
  - combine past and future evidence
- encoder-decoder
  - machine translation
  - question answering
  - dialog

#### 16.2 Recursive Neural Network

Generalize RNN from chains to trees

- weight sharing allows trees to fit variable length data
- useful for graphs, e.g. semantic parsing tree

# 17 Autoencoders

#### 17.1 Overview

Feed-forward neural network for

- compression
- denoising
- sparse representation
- data generation

$$f(x) = z$$
$$g(z) = x$$

# 17.2 Linearity

#### 17.2.1 Linear

f and g are both linear

- hidden node is a compressed representation
- equivalent to PCA if using euclidean norm (squared loss)

$$\min_{W} \frac{1}{2} \sum_{r} \|W_{g}W_{f}x_{n} - x_{n}\|_{2}^{2}$$

# 17.2.2 Non-Linear

f and g are both non-linear

• hidden node is a non-linear manifold

$$\min_{W} \frac{1}{2} \sum_{n} \|g(f(x_n; W_f); W_g) - x_n\|_2^2$$

### 17.3 Deep and Sparse

In theory, one hidden layer is sufficient to represent any possible compression, but in practise more layers is better. When there are more hidden nodes than inputs, use regularization to constrain: e.g. sparsity with a penalty term

$$\min_{W} \frac{1}{2} \sum_{n} \|g(f(x_n; W_f); W_g) - x_n\|_2^2 + c\delta(f(x_n; W_f))$$

where 
$$\delta(f(x_n; W_f)) = \begin{cases} 1, & \text{if } f(x_n; W_f) \neq 0 \\ 0, & \text{if } f(x_n; W_f) = 0 \end{cases}$$

approximate objective is L1 regularization

$$\min_{W} \frac{1}{2} \sum_{n} \|g(f(x_n; W_f); W_g) - x_n\|_2^2 + c \|f(x_n; W_f)\|_1$$

# 17.4 Denoising

Consider  $\tilde{x}$ , the noisy version of input x. Use autoencoder to compress to true representation and reconstruct without noise

$$\min_{W} \frac{1}{2} \sum_{n} \|g(f(\tilde{x}_n; W_f); W_g) - x_n\|_2^2 + c \|f(\tilde{x}_n; W_f)\|_1$$

# 17.5 Probabilistic

Let f and g represent conditional distributions

$$f = Pr(h|x; W_f)$$
$$g = Pr(x|h; W_g)$$

by using sigmoid, softmax, or linear units at the hidden and output layers

#### 17.6 Generative Model

Sample h from some distribution Pr(h) and use the decoder to sample x,  $Pr(x|h;W_q)$ 

# 18 Generative Networks

#### 18.1 Overview

Design a neural network to generate data

- input random noise
- output data

Types

- boltzmann machines
- sigmoid belief networks
- variational autoencoders
- generative adversarial networks
- generative moment matching networks
- sum-product networks

#### 18.2 Variational Autoencoders

#### 18.2.1 Encoder

Train encoder  $P(h|x; W_g)$  to approach simple and fixed distribution (e.g. N(h; 0, I)) so that you can set Pr(h) = N(h; 0, I), objective:

$$\max_{W} \sum_{n} Pr(x_n; W_f, W_g) - cKL(Pr(h|x_n; W_f)||N(h; OI)$$

where KL = Kullback-Liebler divergence

#### 18.2.2 Likelihood

$$Pr(x_n; W_f, W_g) = \int_h Pr(x_n|h; W_g) Pr(h|x_n; W_f) dh$$

since encoder approaches a normal distribution, force it to be gaussian

$$= \int_{h} Pr(x_n|h; W_g) N(h; \mu_n(x_n; W_f), \sigma_n(x_n; W_f) I) dh$$

approximate by a single sample

$$\approx Pr(x_n|h_n; W_g)$$
  
where  $h_n N(h; \mu_n(x_n; W_f), \sigma_n(x_n; W_f)I)$ 

# 18.3 Generative Adversarial Networks

#### 18.3.1 Overview

Two networks:

- 1. generator  $g(z; W_q) \to x$
- 2. discriminator  $d(x; W_d) \to Pr(x \text{ is real})$

Objective

$$\min_{W_g} \max_{W_d} \sum_{n} \log d(x_n; W_d) + \log(1 - d(g(z_n; W_g); W_d))$$

Issues

- one network may dominate the other
- local convergence

#### 18.3.2 Training

for k steps do

sample 
$$z_1 \dots z_m$$
 from  $Pr(z)$   
sample  $x_1 \dots x_m$  from training set

update discriminator with SGD

$$\nabla W_d(\frac{1}{m}\sum_{n=1}^{m}[\log d(x_n; W_d) + \log(1 - d(g(z_n; W_g); W_d))])$$

#### end for

sample  $z_1 \dots z_m$  from Pr(z) update generator with SGD

$$\nabla W_g(\frac{1}{m}\sum_{n=1}^{m}\log(1-d(g(z_n;W_g);W_d)))$$

In the limit, yields

- $Pr(x|z;W_q) \to \text{true data distribution}$
- $Pr(x \text{ is real}; W_d) \rightarrow 0.5$ , real and fake data are indistinguishable

# 19 Ensemble Learning

#### 19.1 Overview

**ensemble learning** method to select and combine ensemble of hypotheses into a better hypothesis, can enlarge hypothesis space

# 19.2 Bagging

bagging majority voting

- each  $h_i$  is wrong with probability p
- the majority of k is wrong with probability  $\sum_{k>n/2} {n \choose k} p^k (1-p)^{n-k}$

weighted majority

• give weight proportional to hypothesis accuracy

#### 19.3 Boosting

**boosting** learn with a weighted training set (more weight = more important) and increase the weight on examples that are misclassified, this can *boost* a weak learner

weak learner produces hypothesis at leas as good as random classifier

Applications

- sensor fusion
- collaborative filtering (Netflix challenge)
- body part recognition (kinect)

#### 19.3.1 Framework

```
set all instance weights w_x = 1

repeat
h_i \leftarrow \text{learn}(\text{dataset, weights})
increase w_x of misclassified examples x
until sufficient number of hypotheses
return weighted majority of h_is with weights w_i proportional to accuracy of h_i
```

#### 19.3.2 Paradigm

- don't try to learn perfect hypothesis, just learn simple rules of thumb and boost them
- good generalization
- principled approach to combine many hypotheses

#### 19.3.3 AdaBoost

```
w_i \leftarrow 1/N \ \forall j
for m=1 \to M do
     h_m \leftarrow \text{learn}(\text{datset}, w)
     err \leftarrow 0
     for each (x_j, y_j) in dataset do
         if h_m(x_i) \neq y_i then
              err \leftarrow err + w_i
         end if
     end for
     for each (x_j, y_j) in dataset do
         if h_m(x_j) = y_j then
              w_j \leftarrow w_j \frac{err}{1-err}
         end if
     end for
     w \leftarrow \text{normalize}(w)
     z_m \leftarrow \log(\frac{1-err}{err})
end for
return weighted - majority(h, z)
```

# 20 Bagging and Distributed Computing

## 20.1 Independent Bagging

 $\begin{tabular}{ll} \textbf{bagging} & combine & independent & classifiers & that were trained on subsets of the dataset (sampling w/o replacement) \\ \end{tabular}$ 

```
bootrap sampling sample subset of datarandom projection sample subset of featuresrandom forest bag of decision trees
```

```
for k = 1 \rightarrow K do

D_k \leftarrow sample data subset

F_k \leftarrow sample feature subset

h_k \leftarrow train classifier based on D_k and F_k

end for

if classification then

return majority(h_1(x) \dots h_K(x))

else if regression then

return average(h_1(x) \dots h_K(x))

end if
```

Kinect: body part recognition

- infrared + gray-scale depth map
- features: depth difference between pairs of pixels
- classification: forest of decision trees

# 20.2 Distributed Computation

"big data" aka large scale machine learning requires distributed computation

- GPU: performing arithmetic operations on all elements of a tensor in parallel
- CPU: train classifiers with a different subset on each core
  - don't combine parameters (e.g. adding together two NN that encode xor doesn't encode xor)
  - combine *predictions* not parameters

# 21 Stream Learning

#### 21.1 Overview

online learning new data continuously arrives

stream learning train as new data arrives

challenges

- can't store all the data, revisit older data
- algorithm must keep up with the stream, process quickly
- patterns may change over time, must be able to update hypothesis on every point or batch

# 21.2 Algorithms

- bayesian learning: lends itself naturally because bayes theorem updates on every example given current state
- optimization-based learning: objective

$$argmin_{\theta} \sum_{n} Loss(x_n, y_n; \theta)$$
  
where  $Loss$  could be  $= -\log Pr(y|x; \theta)$  neg log likelihood  $= [y - h_{\theta}(x)]^2$  squared error

#### 21.3 Gradient Descent

#### Gradient Descent

$$\theta^{(i+1)} \leftarrow \theta^{(i)} - \alpha_i \sum_n \nabla Loss(x_n, y_n; \theta^{(i)})$$
 where  $\alpha \in [0, 1]$  is the learning rate  $n$  indexes data points  $m$  indexes GD iterations

#### Stochastic Gradient Descent

$$\theta^{(n+1)} \leftarrow \theta^{(n)} - \alpha_n \sum_n \nabla Loss(x_n, y_n; \theta^{(n)})$$

where n indexes data points and iterations

Converges if 
$$\sum_{n=1}^{\infty} \alpha_n = \infty$$
 and  $\sum_{n=1}^{\infty} (\alpha_n)^2 < \infty$ 

Adagrad use a different step size for each parameter

$$\theta^{(n+1)} \leftarrow \theta^{(n)} - \frac{\alpha_n}{\tau + \sqrt{s_m^{(n)}}} \frac{\partial Loss(x_n, y_n; \theta^{(n)})}{\partial \theta_m^{(n)}}$$
where  $s_m^{(n)} \leftarrow s_m^{(n-1)} + \left(\frac{\partial Loss(x_n, y_n; \theta^{(n)})}{\partial \theta_m^{(n)}}\right)^2$