# Optimization Methods for Machine Learning

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#### Outline

#### Data Analysis and Machine Learning

- Context
- Applications / Examples, including formulation as optimization problems

# Optimization is being revolutionized by its interactions with machine learning and data analysis.

- new algorithms, and new interest in old algorithms;
- challenging formulations and new paradigms;
- renewed emphasis on certain topics: convex optimization algorithms, complexity, structured nonsmoothness, ...
- many researchers now working on the machine learning / optimization spectrum.

### Data Analysis

Related Terms: Machine Learning, Statistical Inference, Data Mining.

- Extract meaning from data: Understand statistical properties, learn important features and fundamental structures in the data.
- Use this knowledge to make predictions about other, similar data.

Highly multidisciplinary area!

- Foundations in Statistics;
- Computer Science: Al, Machine Learning, Databases, Parallel Systems;
- Optimization provides a toolkit of modeling/formulation and algorithmic techniques.

Modeling and domain-specific knowledge is vital: "80% of data analysis is spent on the process of cleaning and preparing the data." [Dasu and Johnson, 2003].

(Most academic research deals with the other 20%.)

### The Age of "Big Data"

New "Data Science Centers" at many institutions, new degree programs (e.g. Masters in Data Science), new funding initiatives (e.g. NSF's TRIPODS).

- Huge amounts of data are collected, routinely and continuously.
  - Consumer and citizen data: phone calls and text, social media apps, email, surveillance cameras, web activity, online shopping,...
  - Scientific data (particle colliders, satellites, biological / genomic, astronomical,...)
- Affects everyone directly!
- Powerful computers and new specialized architectures make it
  possible to handle larger data sets and analyze them more thoroughly.
- Methodological innovations in some areas. e.g. Deep Learning.
  - Speech recognition in smart phones
  - ▶ AlphaGo: Deep Learning for Go.
  - Image recognition

### Typical Setup

After cleaning and formatting, obtain a data set of m objects:

- Vectors of features:  $a_j$ , j = 1, 2, ..., m.
- Outcome / observation / label  $y_i$  for each feature vector.

#### The outcomes $y_i$ could be:

- a real number: regression
- a label indicating that  $a_j$  lies in one of M classes (for  $M \ge 2$ ): classification
- multiple labels: classify a<sub>i</sub> according to multiple criteria.
- no labels (y<sub>i</sub> is null):
  - subspace identification: Locate low-dimensional subspaces that approximately contain the (high-dimensional) vectors a<sub>i</sub>;
  - clustering: Partition the a<sub>i</sub> into a few clusters.

(Structure may reveal which features in the  $a_j$  are important / distinctive, or enable predictions to be made about new vectors a.)

### Fundamental Data Analysis Task

#### Seek a function $\phi$ that:

- approximately maps  $a_j$  to  $y_j$  for each j:  $\phi(a_j) \approx y_j$  for j = 1, 2, ..., m
- if there are no labels  $y_j$ , or if some labels are missing, seek  $\phi$  that does something useful with the data  $\{a_j\}$ , e.g. assigns each  $a_j$  to an appropriate cluster or subspace.
- satisfies some additional properties simplicity, structure that
  make it "plausible" for the application, robust to perturbations in the
  data, generalizable to other data samples.

Can usually define  $\phi$  in terms of some parameter vector x — thus identification of  $\phi$  becomes a data-fitting problem: Find the best x.

Objective function in this problem often built up of m terms that capture mismatch between predictions and observations for each item of data  $(a_j, y_j)$ .

The process of finding  $\phi$  is called learning or training.

# What's the use of the mapping $\phi$ ?

- Analysis:  $\phi$  especially the parameter x that defines it reveals structure in the data. Examples:
  - Feature selection: reveal the components of vectors  $a_j$  that are most important in determining the outputs  $y_j$ , and quantifies the importance of these features.
  - Uncovers some hidden structure, e.g.
    - ★ finds some low-dimensional subspaces that contain the a<sub>j</sub>;
    - ★ find clusters that contain the a<sub>i</sub>;
    - ★ find a decision tree that builds intuition about how outputs y<sub>j</sub> depend on inputs a<sub>j</sub>.
- Prediction: Given new data vectors  $a_k$ , predict outputs  $y_k \leftarrow \phi(a_k)$ .

### Complications

- noise or errors in  $a_j$  and  $y_j$ . Would like  $\phi$  (and x) to be robust to this. We want the solution to generalize to perturbations of the observed data. Often achieve this via regularized formulations.
- avoid overfitting: Observed data is viewed as an empirical, sampled representation of some underlying reality. Want to avoid overfitting to the particular sample. (Training should produce a similar result for other samples from the same data set.) Again, generalization / regularization.
- missing data: Vectors  $a_j$  may be missing elements (but may still contain useful information).
- missing labels: Some or all  $y_j$  may be missing or null semi-supervised or unsupervised learning.
- online learning: Data  $(a_j, y_j)$  is arriving in a stream rather than all known up-front.

#### Optimization

In optimization, we seek to minimize some objective function by choosing the best values for a set of variables, subject possibly to some constraints on the variables.

The three ingredients — variables, objective function, and constraints — are all important. They can have different characteristics that make the optimization problem easy or hard.

#### The variables could be

- vectors of real numbers;
- ullet vectors of binary variables  $\{0,1\}$  or integers;
- square or rectangular matrices of real numbers;
- functions in a Hilbert space;

or some combination of all of these. Binary and integer variables typically make the problems much harder!

#### The constraints could be

- non-existent: "unconstrained" optimization;
- bounds on the real and integer variables;
- more complicated algebraic expressions or geometric restrictions;
- positive definiteness of the matrix variables:  $X \succeq 0$ ;
- uncertain (depending also on some random variable);
- chance-constrained (e.g. in a list of 100 constraints, want at least 95 of them to be satisfied).

#### The objective function could be

- smooth (multiple-times differentiable);
- nonsmooth but continuous;
- an expectation over some random variable:  $\mathbb{E}_{\xi} f(x; \xi)$  (where x is the optimization variable and  $\xi$  is the random variable).

Some optimization problems have no objective. (In this case we simply seek a point that satisfies the constraints — a *feasible* point.)

#### Optimization Research

#### Optimization research includes

- the process of formulating / modeling practical problems as optimization problems;
- studying the mathematical properties of optimization formulations,
   e.g. sensitivity to uncertainty in their data;
- developing computational algorithms for solving these problems, and studying the mathematical properties of these algorithms;
- developing and testing software that implements these algorithms.

### Application I: Least Squares

$$\min_{x} f(x) := \frac{1}{2} \sum_{j=1}^{m} (a_{j}^{T} x - y_{j})^{2} = \frac{1}{2} ||Ax - y||_{2}^{2}.$$

[Gauss, 1799], [Legendre, 1805]; see [Stigler, 1981].

Here the function mapping data to output is linear:  $\phi(a_j) = a_j^T x$ .

•  $\ell_2$  regularization reduces sensitivity of the solution x to noise in y.

$$\min_{x} \frac{1}{2} ||Ax - y||_{2}^{2} + \lambda ||x||_{2}^{2}.$$

•  $\ell_1$  regularization yields solutions x with few nonzeros:

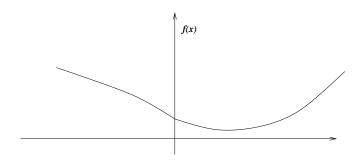
$$\min_{x} \frac{1}{2} ||Ax - y||_{2}^{2} + \lambda ||x||_{1}.$$

Feature selection: Nonzero locations in x indicate important components of  $a_i$ .

• Nonconvex separable regularizers (SCAD, MCP) have nice statistical properties, but lead to nonconvex optimization formulations.

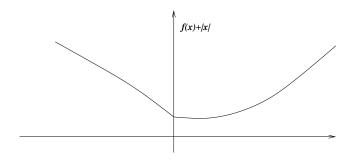
#### $\ell_1$ regularization

Including a multiple of  $||x||_1$  into the objective is a standard way to induce sparsity in the variable vector x.



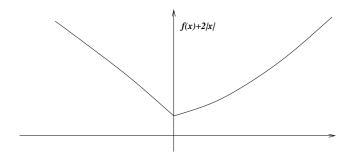
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### Application II: Matrix Completion

Regression over a structured matrix: Observe a matrix X by probing it with linear operators  $A_j(X)$ , giving observations  $y_j$ ,  $j=1,2,\ldots,m$ . Solve a regression problem:

$$\min_{X} \frac{1}{2m} \sum_{j=1}^{m} (A_{j}(X) - y_{j})^{2} = \frac{1}{2m} ||A(X) - y||_{2}^{2}.$$

Each  $A_j$  may observe a single element of X, or a linear combination of elements. Can be represented as a matrix  $A_j$ , so that  $A_j(X) = \langle A_j, X \rangle$ .

Seek the "simplest" X that satisfies the observations. Nuclear-norm (sum-of-singular-values) regularization term induces low rank on X:

$$\min_{X} \frac{1}{2m} \|\mathcal{A}(X) - y\|_2^2 + \lambda \|X\|_*, \quad \text{for some } \lambda > 0.$$

[Recht et al., 2010]

#### **Explicit Low-Rank Parametrization**

Compact, nonconvex formulation is obtained by parametrizing X directly:

$$X = LR^T$$
, where  $L \in \mathbb{R}^{m \times r}$ ,  $R \in \mathbb{R}^{n \times r}$ ,

where r is known (or suspected) rank.

$$\min_{L,R} \frac{1}{2m} \sum_{j=1}^{m} (\mathcal{A}_j(LR^T) - y_j)^2.$$

For symmetric X, have L = R, so  $X = ZZ^T$ , where  $Z \in \mathbb{R}^{n \times r}$ .

(No need for regularizer — rank is hard-wired into the formulation.)

Despite the nonconvexity, near-global minima can be found when  $\mathcal{A}_j$  are incoherent. Use appropriate initialization [Candès et al., 2014], [Zheng and Lafferty, 2015] or the observation that all local minima are near-global [Bhojanapalli et al., 2016].

### Matrix Completion from Individual Entries

When the observations  $A_j$  are of individual elements, recovery is still possible when the true matrix X is itself low-rank and incoherent (i.e. not too "spiky" and with singular vectors randomly oriented).

Need sufficiently many observations [Candès and Recht, 2009].

Procedures based on trimming + truncated singular value decomposition (for initialization) and projected gradient (for refinement) produce good solutions [Keshavan et al., 2010].

### Application III: Nonnegative Matrix Factorization

Given  $m \times n$  matrix Y, seek factors  $L(m \times r)$  and  $R(n \times r)$  that are element-wise positive, such that  $LR^T \approx Y$ .

$$\min_{L,R} \frac{1}{2} ||LR^T - Y||_F^2 \text{ subject to } L \ge 0, R \ge 0.$$

Applications in computer vision, document clustering, chemometrics, ...

Could combine with matrix completion, when not all elements of Y are known, if it makes sense on the application to have nonnegative factors.

If positivity constraint were not present, could solve this in closed form with an SVD, since Y is observed completely.

### Application IV: Sparse Inverse Covariance

Let  $Z \in \mathbb{R}^p$  be a (vector) random variable with zero mean. Let  $z_1, z_2, \ldots, z_N$  be samples of Z. Sample covariance matrix (estimates covariance between components of Z):

$$S := \frac{1}{N-1} \sum_{\ell=1}^{N} z_{\ell} z_{\ell}^{\mathsf{T}}.$$

Seek a sparse inverse covariance matrix:  $X \approx S^{-1}$ .

X reveals dependencies between components of Z:  $X_{ij} = 0$  if the i and j components of Z are conditionally independent.

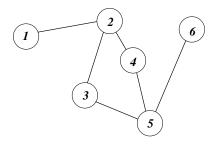
Can the relationship between components i and j be predicted if we know all the other variables, or is there some direct aspect to the relationship that cannot be predicted?

Obtain X from the regularized formulation:

$$\min_{X} \left\langle S, X \right\rangle - \log \det(X) + \lambda \|X\|_1, \quad \text{where } \|X\|_1 = \sum_{i,j} |X_{ij}|.$$

[d'Aspremont et al., 2008, Friedman et al., 2008].

### Reveals Network Structure. Example with p = 6.



$$X = \begin{bmatrix} * & * & 0 & 0 & 0 & 0 \\ * & * & * & * & 0 & 0 \\ 0 & * & * & 0 & * & 0 \\ 0 & * & 0 & * & * & 0 \\ 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * \end{bmatrix}$$

# Application V: Sparse Principal Components (PCA)

Seek sparse approximations to the leading eigenvectors of the sample covariance matrix S.

For the leading sparse principal component, solve

$$\max_{v \in \mathbb{R}^n} v^T S v = \langle S, v v^T \rangle \quad \text{s.t. } \|v\|_2 = 1, \ \|v\|_0 \leq k,$$

for some given  $k \in \{1, 2, ..., n\}$ . Convex relaxation replaces  $vv^T$  by an  $n \times n$  positive semidefinite proxy M:

$$\max_{M \in \mathbb{SR}^{n \times n}} \langle S, M \rangle \quad \text{s.t. } M \succeq 0, \ \langle I, M \rangle = 1, \ \|M\|_1 \leq R,$$

where  $|\cdot|_1$  is the sum of absolute values [d'Aspremont et al., 2007].

Adjust the parameter R to obtain desired sparsity.

# Sparse PCA (rank r)

For sparse leading rank-r eigenspace, seek  $V \in \mathbb{R}^{n \times r}$  with orthonormal columns such that  $\langle S, VV^T \rangle$  is maximized, and V has at most k nonzero rows. Convex relaxation:

$$\max_{M \in S\mathbb{R}^{n \times n}} \left\langle S, M \right\rangle \quad \text{s.t. } 0 \preceq M \preceq I, \ \left\langle I, M \right\rangle \leq r, \ \|M\|_1 \leq R.$$

Explicit low-rank formulation is

$$\max_{F \in \mathbb{R}^{n \times r}} \langle S, FF^T \rangle \quad \text{s.t. } \|F\|_2 \le 1, \ \|F\|_{2,1} \le \bar{R},$$

where  $||F||_{2,1} := \sum_{i=1}^{n} ||F_{i\cdot}||_{2}$ .

[Chen and Wainwright, 2015]

### Application VI: Sparse + Low-Rank

Given  $Y \in \mathbb{R}^{m \times n}$ , seek low-rank M and sparse S such that  $M + S \approx Y$ .

#### Applications:

- Robust PCA: Sparse *S* represents "outlier" observations.
- Foreground-Background separation in video processing.
  - ► Each column of *Y* is one frame of video, each row is a single pixel evolving in time.
  - ► Low-rank part *M* represents background, sparse part *S* represents foreground.

#### Convex formulation:

$$\min_{M,S} \|M\|_* + \lambda \|S\|_1$$
 s.t.  $Y = M + S$ .

[Candès et al., 2011, Chandrasekaran et al., 2011]

#### Sparse + Low-Rank: Compact Formulation

Compact formulation: Variables  $L \in \mathbb{R}^{n \times r}$ ,  $R \in \mathbb{R}^{m \times r}$ ,  $S \in \mathbb{R}^{m \times n}$  sparse.

$$\begin{split} & \min_{L,R,S} \frac{1}{2} \|LR^T + S - Y\|_F^2 + \lambda \|S\|_1 \quad \text{(fully observed)} \\ & \min_{L,R,S} \frac{1}{2} \|P_{\Phi}(LR^T + S - Y)\|_F^2 + \lambda \|S\|_1 \quad \text{(partially observed),} \end{split}$$

where  $\Phi$  represents the locations of the observed entries.

[Chen and Wainwright, 2015, Yi et al., 2016].

(For well-posedness, need to assume that the "true" L, R, S satisfy certain incoherence properties.)

# Application VII: Subspace Identification

Given vectors  $a_j \in R^n$  with missing entries, find a subspace of  $\mathbb{R}^n$  such that all "completed" vectors  $a_j$  lie approximately in this subspace.

If  $\Omega_j \subset \{1,2,\ldots,n\}$  is the set of observed elements in  $a_j$ , seek  $X \in \mathbb{R}^{n \times d}$  such that

$$[a_j-Xs_j]_{\Omega_j}\approx 0,$$

for some  $s_j \in \mathbb{R}^d$  and all  $j = 1, 2, \ldots$  [Balzano et al., 2010, Balzano and Wright, 2014].

**Application:** Structure from motion. Reconstruct opaque object from planar projections of surface reference points.









# Application VIII: Linear Support Vector Machines

Each item of data belongs to one of two classes:  $y_i = +1$  and  $y_i = -1$ .

Seek  $(x, \beta)$  such that

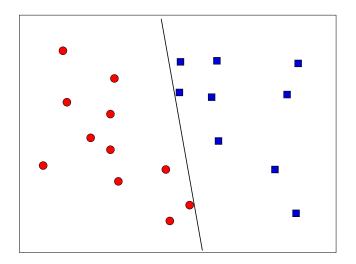
$$a_j^T x - \beta \ge 1$$
 when  $y_j = +1$ ;  $a_j^T x - \beta \le -1$  when  $y_j = -1$ .

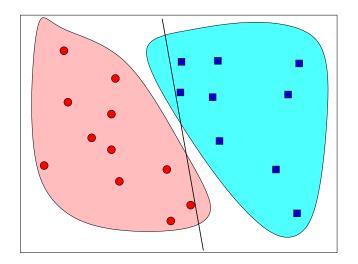
The mapping is  $\phi(a_j) = \operatorname{sign}(a_i^T x - \beta)$ .

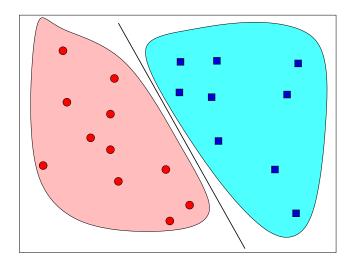
Design an objective so that the *j*th loss term is zero when  $\phi(a_j) = y_j$ , positive otherwise. A popular one is hinge loss:

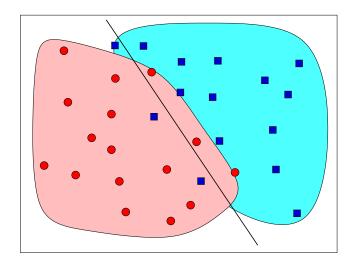
$$H(x) = \frac{1}{m} \sum_{j=1}^{m} \max(1 - y_j(a_j^T x - \beta), 0).$$

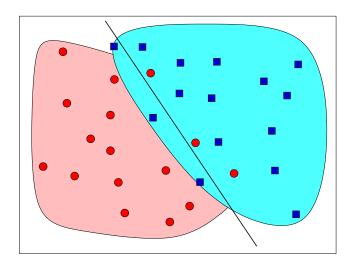
Add a regularization term  $(\lambda/2)\|x\|_2^2$  for some  $\lambda > 0$  to maximize the margin between the classes.











### Application IX: Nonlinear SVM

Data  $a_j$ ,  $j=1,2,\ldots,m$  may not be *separable* neatly into two classes  $y_j=+1$  and  $y_j=-1$ . Apply a nonlinear transformation  $a_j\to\psi(a_j)$  ("lifting") to make separation more effective. Seek  $(x,\beta)$  such that

$$\psi(a_j)^T x - \beta \ge 1$$
 when  $y_j = +1$ ;  
 $\psi(a_j)^T x - \beta \le -1$  when  $y_j = -1$ .

Leads to the formulation:

$$\min_{x} \frac{1}{m} \sum_{j=1}^{m} \max(1 - y_{j}(\psi(a_{j})^{T}x - \beta), 0) + \frac{1}{2}\lambda ||x||_{2}^{2}.$$

Can avoid defining  $\psi$  explicitly by using instead the dual of this QP.

#### Nonlinear SVM: Dual

Dual is a quadratic program in m variables, with simple constraints:

$$\min_{\alpha \in \mathbb{R}^m} \frac{1}{2} \alpha^T Q \alpha - e^T \alpha \text{ s.t. } 0 \le \alpha \le (1/\lambda)e, \ y^T \alpha = 0.$$

where 
$$Q_{k\ell} = y_k y_\ell \psi(a_k)^T \psi(a_\ell)$$
,  $y = (y_1, y_2, \dots, y_m)^T$ ,  $e = (1, 1, \dots, 1)^T$ .

No need to choose  $\psi(\cdot)$  explicitly. Instead choose a kernel K, such that

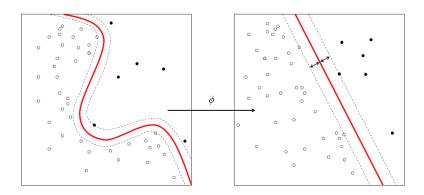
$$K(a_k, a_\ell) \sim \psi(a_k)^T \psi(a_\ell).$$

[Boser et al., 1992, Cortes and Vapnik, 1995]. "Kernel trick."

Gaussian kernels are popular:

$$K(a_k, a_\ell) = \exp(-\|a_k - a_\ell\|^2/(2\sigma)),$$
 for some  $\sigma > 0$ .

### Nonlinear SVM



## Application X: Logistic Regression

Binary logistic regression is similar to binary SVM, except that we seek a function p that gives odds of data vector a being in class 1 or class 2, rather than making a simple prediction.

Seek odds function p parametrized by  $x \in \mathbb{R}^n$ :

$$p(a;x) := (1 + e^{a^T x})^{-1}.$$

Choose x so that  $p(a_j; x) \approx 1$  when  $y_j = 1$  and  $p(a_j; x) \approx 0$  when  $y_j = 2$ .

Choose *x* to minimize a negative log likelihood function:

$$\mathcal{L}(x) = -\frac{1}{m} \left[ \sum_{y_j=2} \log(1 - p(a_j; x)) + \sum_{y_j=1} \log p(a_j; x) \right]$$

Sparse solutions x are interesting because the indicate which components of  $a_j$  are critical to classification. Can solve:  $\min_z \mathcal{L}(z) + \lambda ||z||_1$ .

### Multiclass Logistic Regression

Have M classes instead of just 2. M can be large e.g. identify phonemes in speech, identify line outages in a power grid.

Labels  $y_{j\ell}=1$  if data point j is in class  $\ell;\ y_{j\ell}=0$  otherwise;  $\ell=1,\ldots,M.$ 

Find subvectors  $x_{[\ell]}$ ,  $\ell=1,2,\ldots,M$  such that if  $a_j$  is in class k we have

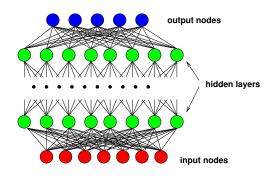
$$a_j^T x_{[k]} \gg a_j^T x_{[\ell]}$$
 for all  $\ell \neq k$ .

Find  $x_{[\ell]}$ ,  $\ell=1,2,\ldots,M$  by minimizing a negative log-likelihood function:

$$f(x) = -\frac{1}{m} \sum_{j=1}^{m} \left[ \sum_{\ell=1}^{M} y_{j\ell} (a_j^T x_{[\ell]}) - \log \left( \sum_{\ell=1}^{M} \exp(a_j^T x_{[\ell]}) \right) \right]$$

Can use group LASSO regularization terms to select important features from the vectors  $a_j$ , by imposing a common sparsity pattern on all  $x_{[\ell]}$ .

# Application XI: Deep Learning



Inputs are the vectors  $a_j$ , outputs are odds of  $a_j$  belonging to each class (as in multiclass logistic regression).

At each layer, inputs are converted to outputs by a linear transformation composed with an element-wise function:

$$a^{\ell+1} = \sigma(W^{\ell}a^{\ell} + g^{\ell}),$$

where  $a^{\ell}$  is node values at layer  $\ell$ ,  $(W^{\ell}, g^{\ell})$  are parameters in the network,  $\sigma$  is the element-wise function.

## Deep Learning

The element-wise function  $\sigma$  makes transformations to scalar input:

- Logistic function:  $t \to 1/(1+e^{-t})$ ;
- Hinge:  $t \rightarrow \max(t, 0)$ : "ReLU";
- Bernoulli: random!  $t \to 1$  with probability  $1/(1 + e^{-t})$  and  $t \to 0$  otherwise (inspired by neuron behavior).

The example depicted shows a completely connected network — but more typically networks are engineered to the application (speech processing, object recognition, ...).

- local aggregation of inputs: pooling;
- restricted connectivity + constraints on weights (elements of  $W^{\ell}$  matrices): convolutions.

## Training Deep Learning Networks

The network contains many parameters —  $(W^{\ell}, g^{\ell})$ ,  $\ell = 1, 2, ..., L$  in the notation above — that must be selected by training on the data  $(a_j, y_j)$ , j = 1, 2, ..., m.

Objective has the form:

$$\sum_{j=1}^m h(x;a_j,y_j)$$

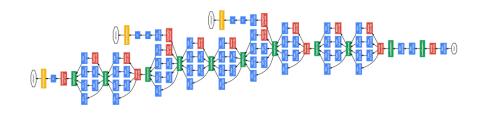
where  $x = (W^1, g^1, W^2, g^2, ...)$  are the parameters in the model and h measures the mismatch between observed output  $y_j$  and the outputs produced by the model (as in multiclass logistic regression).

Nonlinear, Nonconvex. It's also random in some cases (but then we can work with expectation).

Composition of many simple functions.

### GoogLeNet

Visual object recognition: Google's prize-winning network from 2014 [Szegedy et al., 2015].



### How Does a Neural Network Make The Problem Easier?

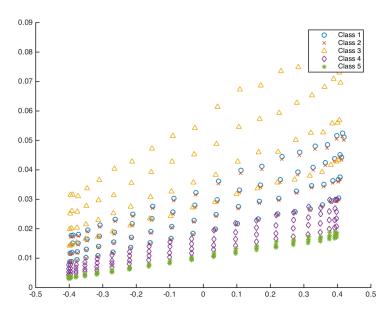
Can think of the neural network as transforming the raw data in a way that makes the ultimate task (regression, classification) easier.

We consider a multiclass classification application in power systems. The raw data is PMU measurements at different points in a power grid, under different operating conditions. The goal is to use this data to detect line outages. Each class corresponds to outage of a particular line.

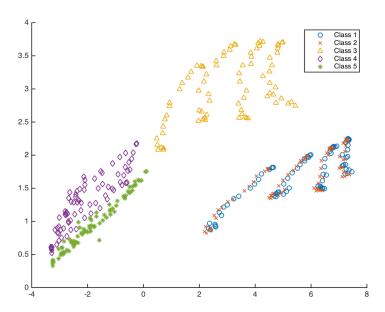
High-dimensional. Can illustrate by doing a singular value decomposition of the data matrix and plotting pairs of principal components on a 2-d graph.

Do this before and after transformation. One hidden layer with 200 nodes.

### Raw Data (Before Transformation)



## After Transformation by One Layer



### Summary

Optimization provides powerful frameworks for formulating and solving problems in data analysis and machine learning.

BUT it's usually not enough to just formulate these problems and use off-the-shelf optimization technology to solve them. The algorithms need to be customized to the problem structure (in particular, large amount of data) and the context.

Research in this area has exploded over the past decade and is still going strong.

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