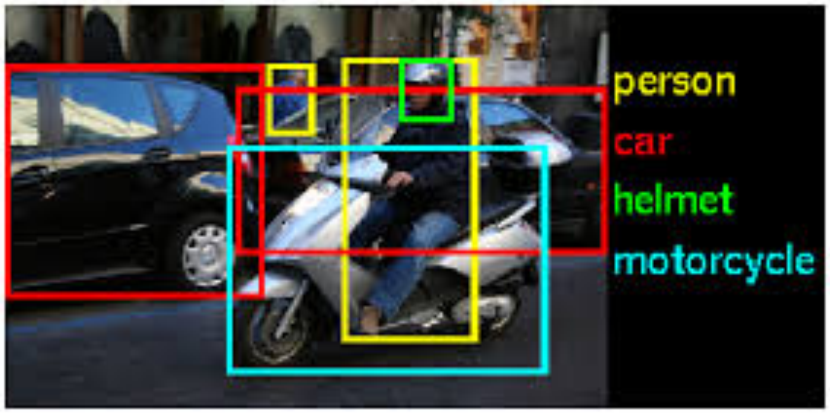
Optimization Methods for Supervised Machine Learning: From Linear Models to Deep Learning. Part I

Katya Scheinberg
jointly with Frank Curtis
LEHIGH UNIVERSITY

ML applications

- Computer vision
- Machine translation
- Speech recognition
- Text categorization
- Recommender systems
- Ranking web search results
- Next word prediction
- Video content classification
- Anomaly detection

Popular applications of deep learning models



Data on Google scale today

- ImageNet Large Scale Visual Recognition Competition: **1.2 million 224x224 images**
- **300** hours of video are uploaded to YouTube every minute! **819,417,600** hours of video total **> 93,000 years**.
- Google's big initiative is: **next billion users**.
  - Next word prediction in texts.
  - Machine translation
  - Image classification and recognition

LEARNING PROBLEM, SETUP

Supervised learning problem

- Given a sample data set S of n (input, label) pairs, written

$$S = \{(x_1, y_1), \ldots, (x_n, y_n)\}.$$

- each pair is an observation of the random variables (x, y) with some unknown distribution $P(x, y)$ over $\mathcal{X}, \mathcal{Y}$.

- each pair (x_i, y_i) is an independent sample

- Find a hypothesis (predictor) $p(w, \cdot)$ such that $p(w, x) \approx y$, i.e.,

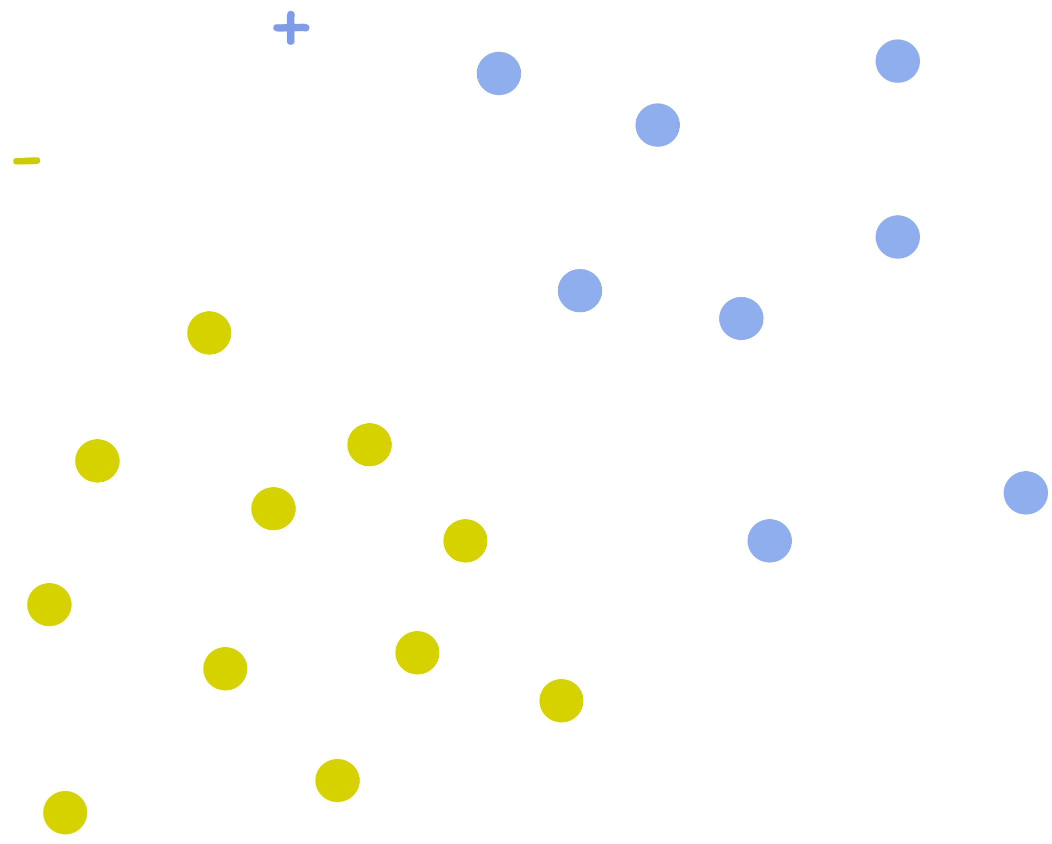
$$\max_w \int_{\mathcal{X}\times\mathcal{Y}} \mathbb{1}[p(w, x) \approx y] dP(x, y).$$

For example, *x* is the image of a letter and *y* is the letter label.
What should *p(w,x)* be?

Binary classification problem

$Y \in \{-1,+1\}$

Two sets of
labeled points



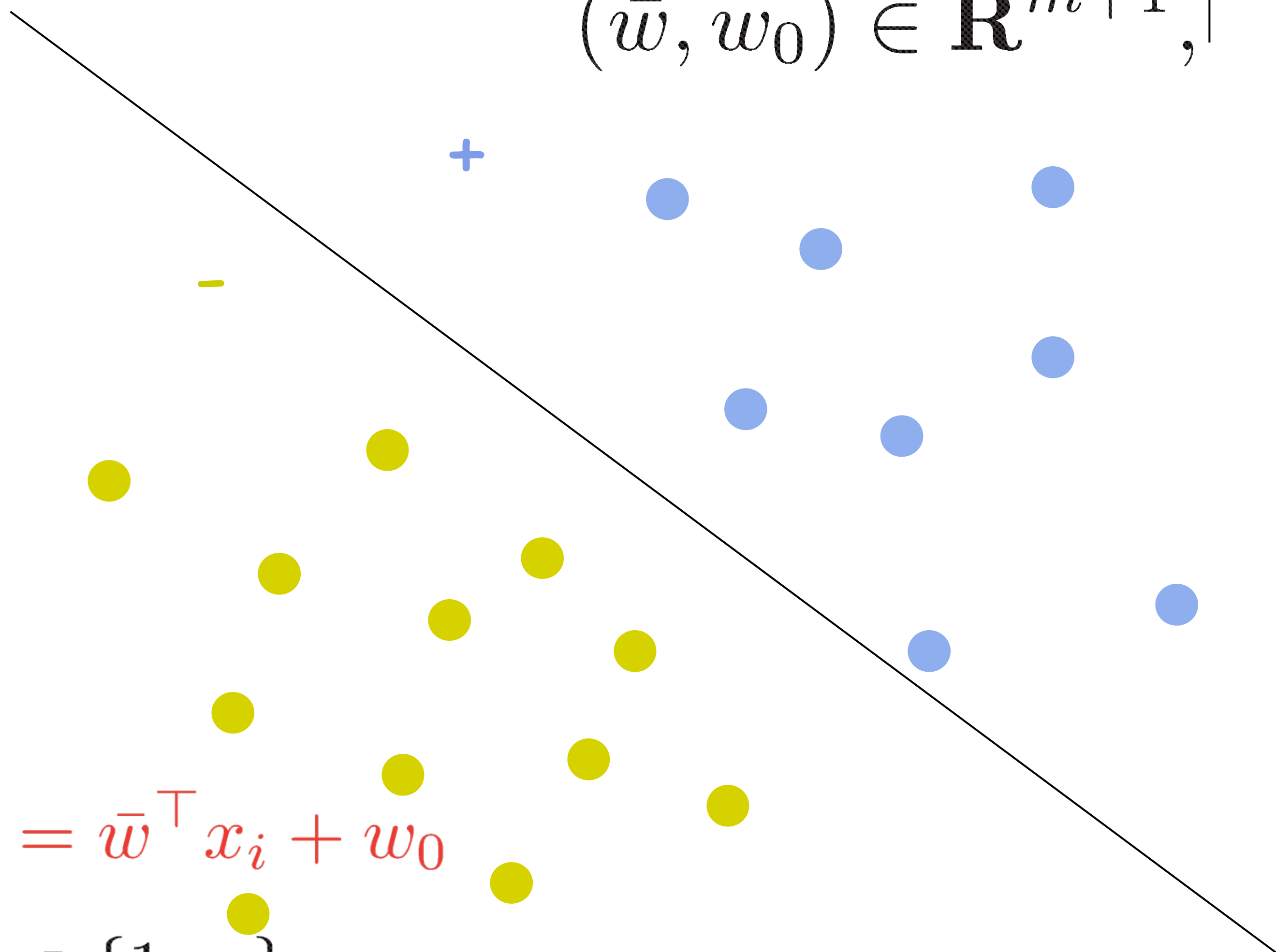
Linear classifier

y∈ {-1,+1}

$$\bar{w}^\top x + w_0 = 0$$

$$(\bar{w}, w_0) \in \mathbf{R}^{m+1},$$

Like this:



$$p(w, x_i) = \bar{w}^\top x_i + w_0$$

$$\forall i \in \{1..n\}$$

Binary Classification Objective

Expected risk: ideal objective

$$\max_{w} \int_{\mathcal{X}\times\mathcal{Y}} \mathbb{1}[yp(w,x) > 0] dP(x,y).$$

$\Updownarrow$

$$\min_{w} f_{01}(w) = \mathbb{E}[\ell_{01}(p(w,x),y)]$$

$$\ell_{01}(p(w,x),y) = \begin{cases} 0 & \text{if } yp(w,x) > 0 \\ 1 & \text{if } yp(w,x) \leq 0, \end{cases}$$

Usually an intractable problem

Binary Classification Objective

Expected risk: ideal objective

$$\max_{w} \int_{\mathcal{X}\times\mathcal{Y}} \mathbb{1}[yp(w,x) > 0]dP(x,y).$$

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Empirical risk: realizable objective

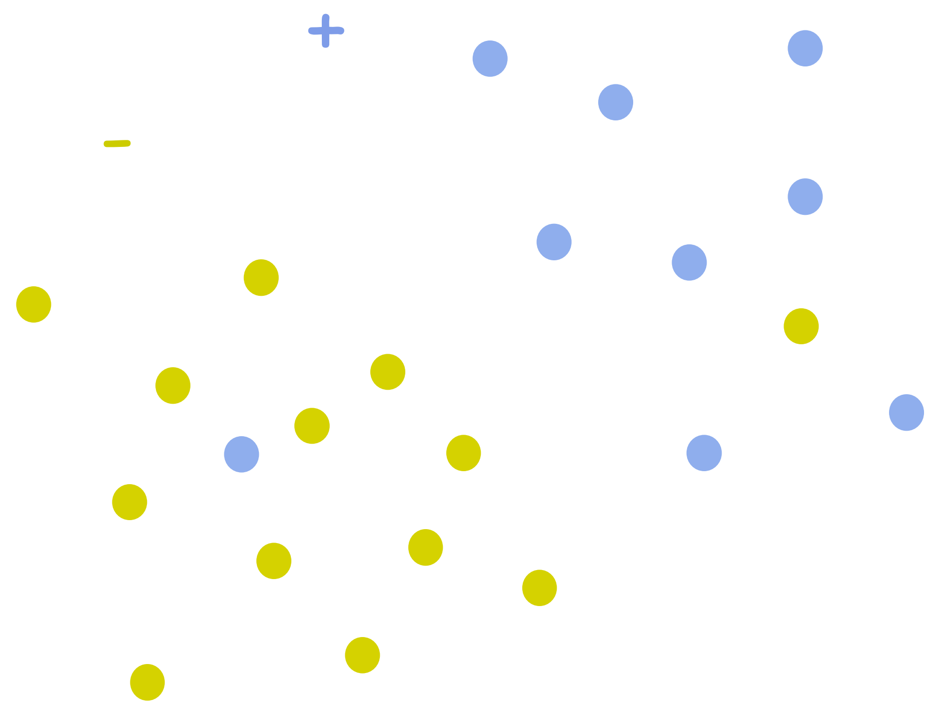
$$\min_{w} \hat{f}_{01}(w) = \frac{1}{n}\sum\nolimits_{i=1}^{n} \ell_{01}(p(w,x_i),y_i)$$

Finite, but NP hard problem

Handling outliers, logistic regression

$$\ln\left(\frac{P(Y=y|x)}{1-P(Y=y|x)}\right) = yp(w,x).$$

$$P(Y=y|x) = \frac{e^{yp(w,x)}}{1+e^{yp(w,x)}} = \frac{1}{1+e^{-yp(w,x)}}. \quad (1)$$



Logistic Regression Model

Expected loss: ideal objective

$$\min_{w} \; f(w) = \int_{\mathcal{X}\times\mathcal{Y}} \ell(p(w,x),y)dP(x,y) = \mathbb{E}[\ell(p(w,x),y)], \qquad (1)$$

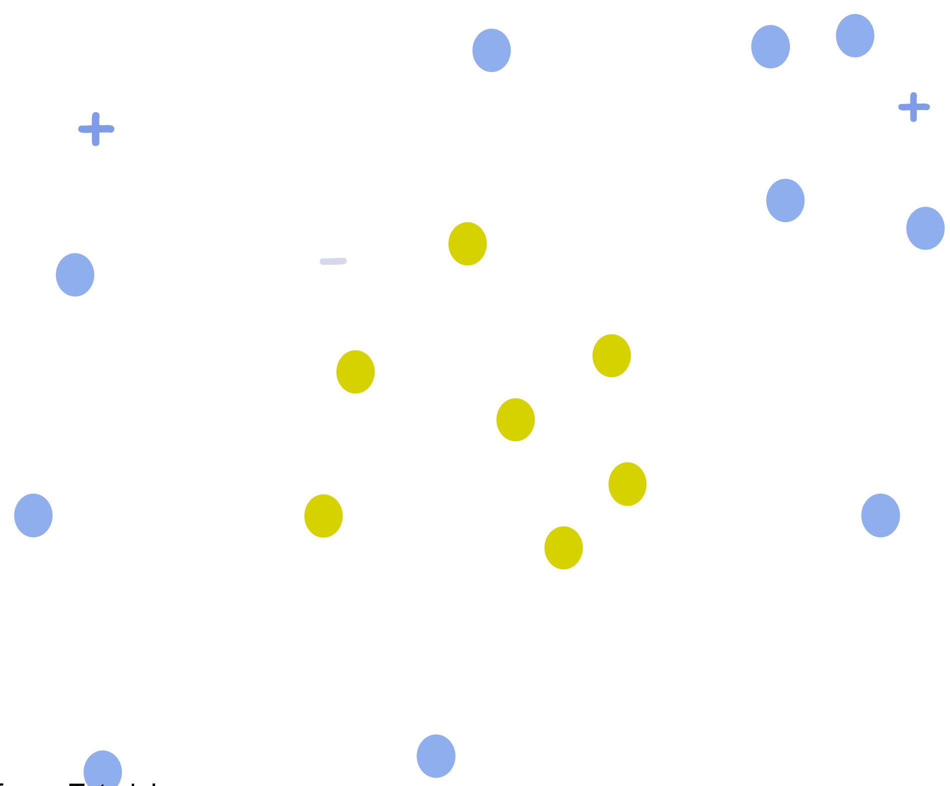
$$\ell(p(w,x),y) = \log(1+e^{-yp(w,x)}).$$

Empirical loss: realizable objective

$$\min_{w} \hat{f}(w) = \frac{1}{n}\sum_{i=1}^{n} \log(1+e^{-yp(w,x)})$$

This is a convex function when *p(w,x)* is linear in *w*

Linear classifier, generalization



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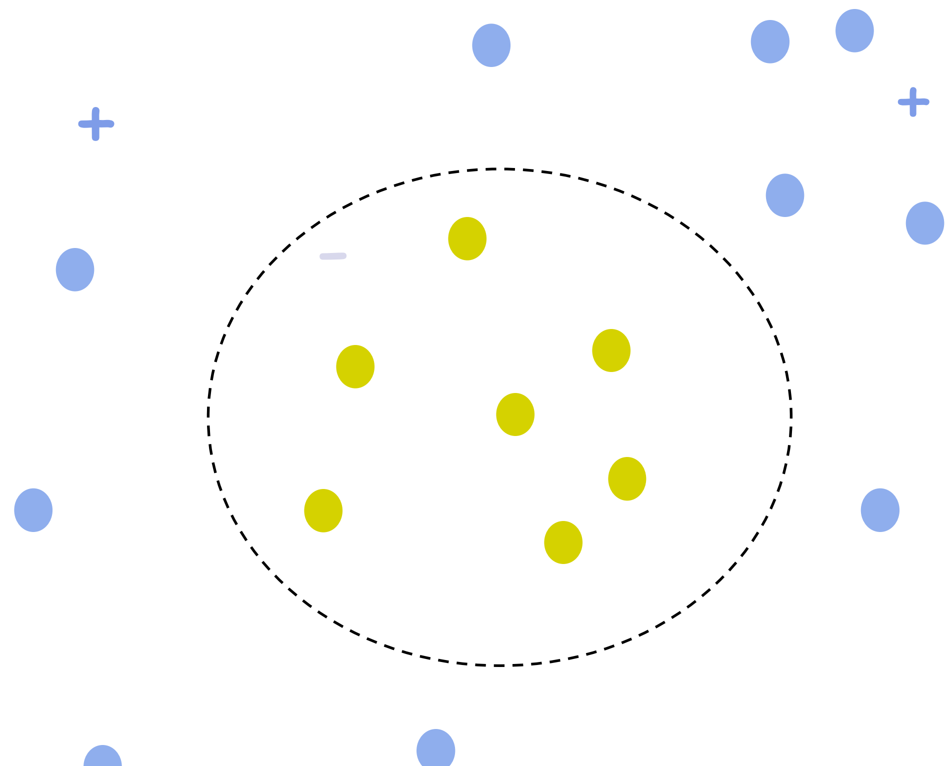
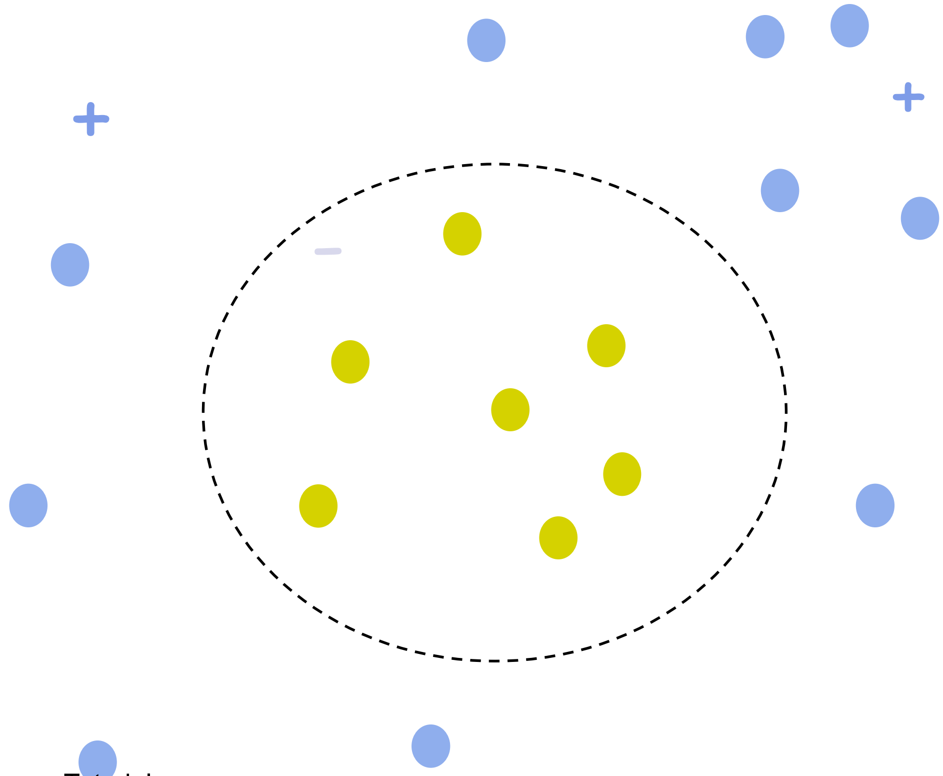


Linear classifier, generalization

$$w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_1 x_2 + w_5 x_2^2 + w_0$$

$$\bar{w}^\top \phi(x) + w_0, \;\; \phi(x) = (x_1, x_2, x_1^2, x_1 x_2, x_2^2) \in \mathbf{R}^5$$



Learning guarantees

$$\hat{w}_{opt} = \arg\min_{w \in R^m} \hat{f}(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w, x_i), y_i)$$

Problem is well defined, even if it may be difficult to solve

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However, we are really interested in

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$$w_{opt} = \arg\min_{w} f(w) = \mathbb{E}[\ell(p(w, x), y)]$$

How does $\hat{w}_{opt}$ behave on the unseen data?

$$|\mathbb{E}[\ell(p(w_{opt}, x), y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(p(w_{opt}, x_i), y_i)| \leq O\left(\sqrt{\frac{\mathcal{C}(p(\cdot,\cdot))}{n}}\right)$$

$\mathcal{C}(p(\cdot,\cdot))$ is a measure of complexity of the class of predictors

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$$w_{opt} = \arg\min_{w} f(w) = \mathbb{E}[\ell(p(w, x), y)]$$

How do $\hat{w}_{opt}$ and w_{opt} relate?

$$|\mathbb{E}[\ell(p(w_{opt}, x), y] - \mathbb{E}[\ell(p(\hat{w}_{opt}, x), y)]| \leq O\left(\sqrt{\frac{\mathcal{C}(p(\cdot, \cdot))}{n}}\right)$$

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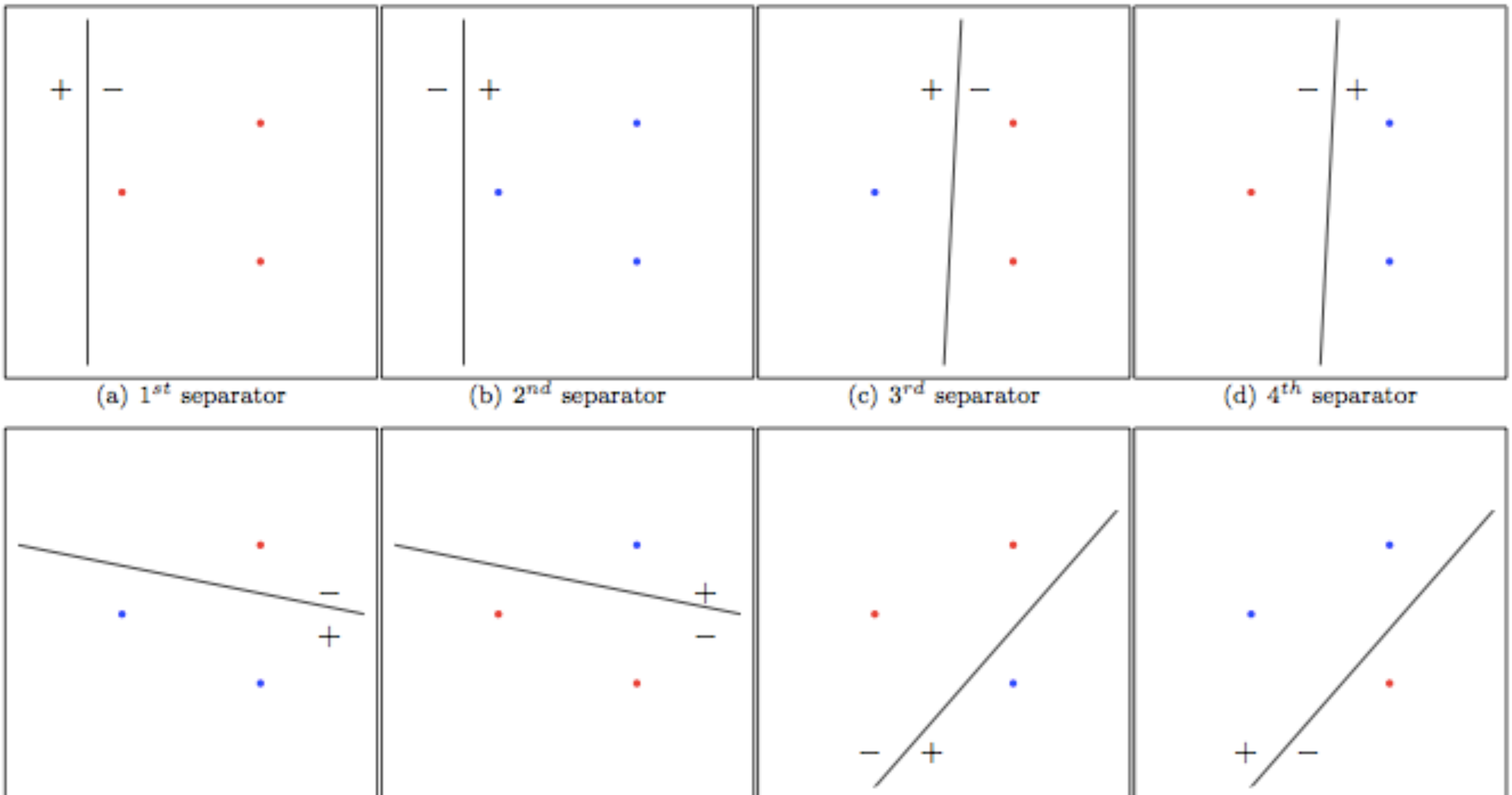
Learning guarantees via Vapnik-Chervonenkis (VC)-dimension

$$|\mathbb{E}[\ell_{01}(p(w,x),y] - \sum_{i=1}^{n} \ell_{01}(p(w,x_i),y_i)| \leq O\left(\sqrt{\frac{VC(p(\cdot,\cdot))}{n}}\right)$$

- ***VC(p(·,·)*** **- VC dimension of a set of classifiers – is the maximum number of points** ***x*** **such that any labeling can be separated by a classifier from this set.**

Vapnik-Chervonenkis (VC)-dimension, example



(a) 1^{st} separator (b) 2^{nd} separator (c) 3^{rd} separator (d) 4^{th} separator

(e) 5^{th} separator (f) 6^{th} separator (g) 7^{th} separator (h) 8^{th} separator

Learning guarantees via Vapnik-Chervonenkis (VC)-dimension

$$|\mathbb{E}[\ell_{01}(p(w,x),y] - \sum_{i=1}^{n} \ell_{01}(p(w,x_i),y_i)| \leq O\left(\sqrt{\frac{VC(p(\cdot,\cdot))}{n}}\right)$$

- *VC(p(·,·)* - VC dimension of a set of classifiers – is the maximum number of points *x* such that any labeling can be separated by a classifier from this set.
- VC(linear classifiers) = *m+1*
- Conclusion: large dimension of w require large data sets.

OPTIMIZATION METHODS FOR LOGISTIC REGRESSION

Gradient descent with line search

$$\min_{w \in \mathbf{R}^m} F(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w, x_i), y_i) = \frac{1}{n}\sum_{i=1}^{n} f_i(w)$$

$$\nabla F(w_k) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(w) \tag{1}$$

Algorithm 1 Gradient descent with line search

Parameters: the intial step size α_0, backtracking parameter $\gamma \in (0,1)$.
Initialize: w_0
Iterate:
for $k = 1, 2, \ldots$ **do**
  for $j = 0, 1, 2, \ldots$ **do**
    $w_{k+1} = w_k - \gamma^j \alpha_0 \nabla F(w_k)$
    Compute $F(w_k)$, if it satifies sufficient decrease condition, then **Break**
  end for
end for

Gradient descent with line search

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Convergence rate *$O(\log(1/\epsilon))$* (strongly convex case)

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Stochastic Gradient Descent

Choose a subset of *{1, ⋯, n}*, $S_{k,}$ uniformly at random

$$\nabla_{S_k} F(w_k) = \frac{1}{|S_k|} \sum_{i \in S_k} \nabla f_i(x)$$

$$\mathbb{E}[\nabla_{S_k} F(w_k)] = \nabla F(w_k)$$

Parameters: the step size sequence $\eta_k > 0$ and the minibatch size s
Initialize: w_0
for $k = 1, 2, \ldots$ **do**
  Generate S_k, $|S_k| = s$, uniformly from $\{1, \ldots, n\}$
  $w_{k+1} = w_k - \eta_k \nabla_{S_k} F(w_k)$
end for

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end for

Convergence rate *O(1/*ϵ*)* (strongly convex case)

Work per-iteration is O(sm)<<O(nm), but convergence sensitive to η_k and *s*

Stochastic Gradient Descent with Momentum

Parameters: learning rate $\eta > 0$; momentum weight $\theta \in (0,1)$; mini-batch size $s \in \mathbb{N}$

Initialize: $w_0 \in R^n$; $v_0 = 0 \in R^n$

for $k = 1, 2, \ldots$ **do**

  Generate S_k with $|S_k| = s$ uniformly from $\{1, \ldots, n\}$

  Set $v_k \leftarrow \theta v_{k-1} + \nabla_{S_k} F(w_k)$

  Set $w_{k+1} \leftarrow w_k - \eta v_k$

end for

Work per-iteration is O(sm), less sensitive to η but no convergence theory

Stochastic Variance Reducing Gradient method

Parameters: learning rate $\eta > 0$; mini-batch size $s \in \mathbb{N}$; inner loop size $m \in \mathbb{N}$

Initialize: $\tilde{w}_0 \in R^n$

for $k = 1, 2, \ldots$ **do** — Outer Loop

  Set $w_0 \leftarrow \tilde{w}_{k-1}$

  Set $v_0 \leftarrow \nabla F(w_0)$

  Set $w_1 \leftarrow w_0 - \eta v_0$

  for $t = 1, \ldots, m-1$ **do** — Inner Loop

    Generate S_t with $|S_t| = s$ uniformly from $\{1, \ldots, n\}$

    Set $v_t \leftarrow \nabla_{S_t} F(w_t) - \nabla_{S_t} F(w_0) + v_0$

    Set $w_{t+1} \leftarrow w_t - \eta v_t$

  end for

  Set $\tilde{w}_k = w_t$ with t chosen uniformly from $\{0, \ldots, m\}$

end for

[Johnson & Zhang, 2013]

SARAH (momentum version of SVRG)

Parameters: learning rate $\eta > 0$; mini-batch size $s \in \mathbb{N}$; inner loop size $m \in \mathbb{N}$

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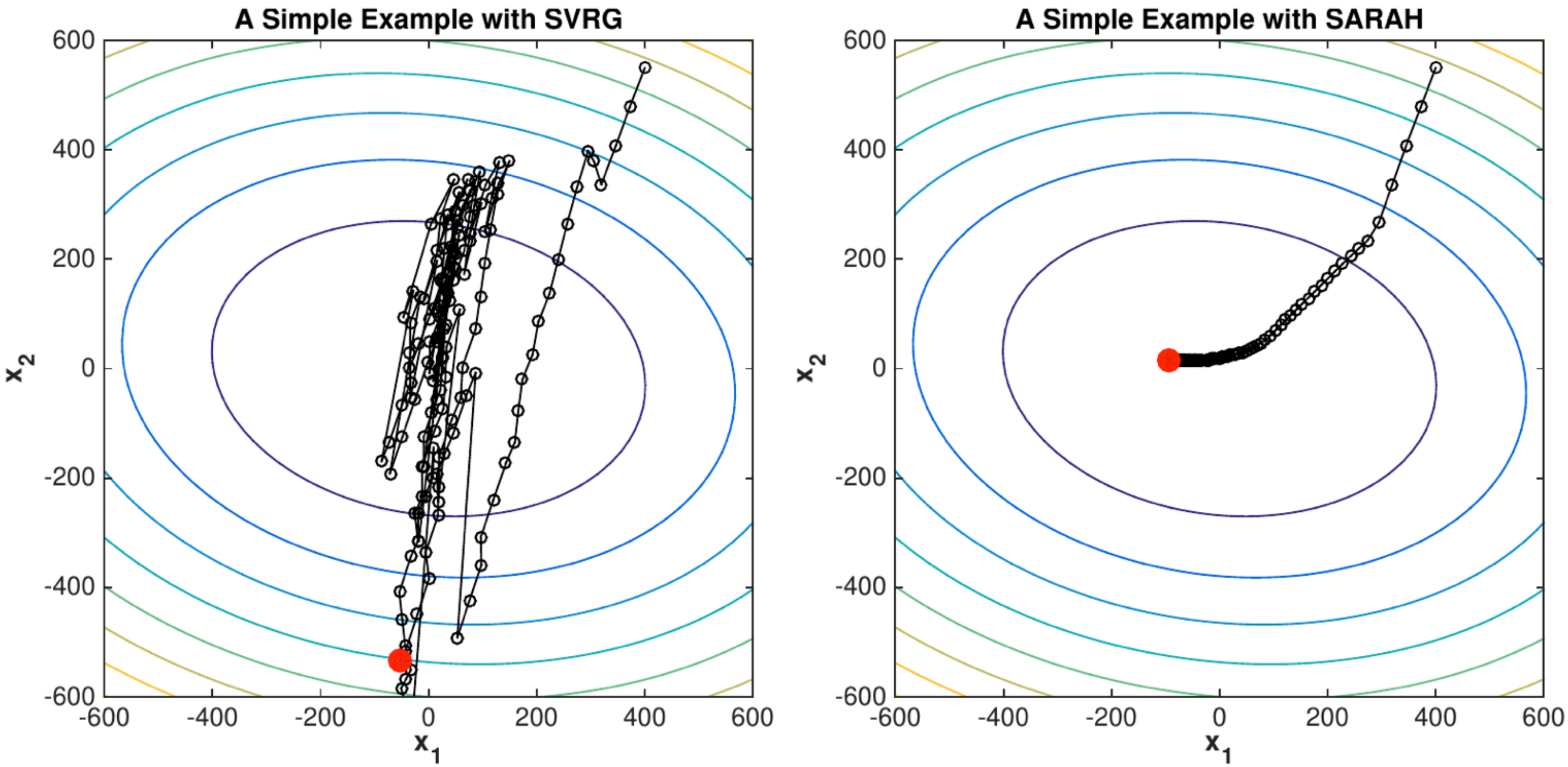
[Nguyen, Liu, S & Takac, 2017]

Regular SG vs. Momentum SG



Convergence rates comparisons

For strongly convex functions, κ is the condition number

Method	Complexity
GD	$\mathcal{O}\left(n\kappa \log\left(1/\epsilon\right)\right)$
SGD	$\mathcal{O}\left(1/\epsilon\right)$
SVRG	$\mathcal{O}\left(\left(n+\kappa\right)\log\left(1/\epsilon\right)\right)$
SARAH	$\mathcal{O}\left(\left(n+\kappa\right)\log\left(1/\epsilon\right)\right)$

For convex functions

Method	Complexity
GD	$\mathcal{O}\left(n/\epsilon\right)$
SGD	$\mathcal{O}\left(1/\epsilon^2\right)$
SVRG	$\mathcal{O}\left(n+\left(\sqrt{n}/\epsilon\right)\right)$
SARAH	$\mathcal{O}\left(\left(n+\left(1/\epsilon\right)\right)\log(1/\epsilon)\right)$

What's so good about stochastic gradient method?

$$\hat{w}_{opt} = \arg\min_{w \in R^m} \hat{f}(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(p(w, x_i), y_i)$$

$$w_{opt} = \arg\min_{w} f(w) = \mathbb{E}[\ell(p(w, x), y)]$$

$$\hat{w}_\epsilon : \hat{f}(w_\epsilon) - \hat{f}(\hat{w}_{opt}) \leq \epsilon$$

$$\begin{aligned} |\hat{f}(\hat{w}_\epsilon) - f(w_{opt})| &\leq |\hat{f}(\hat{w}_\epsilon) - f(\hat{w}_\epsilon)| \\ &+ |\hat{f}(\hat{w}_\epsilon) - \hat{f}(\hat{w}_{opt})| \\ &+ |\hat{f}(\hat{w}_{opt}) - f(\hat{w}_{opt})| \\ &+ |f(\hat{w}_{opt}) - f(w_{opt})|. \end{aligned}$$

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$$\begin{aligned} |\hat{f}(\hat{w}_\epsilon) - f(w_{opt})| &\leq O\left(\frac{1}{\sqrt{n}}\right) \\ &+ \epsilon \\ &+ O\left(\frac{1}{\sqrt{n}}\right) \\ &+ O\left(\frac{1}{\sqrt{n}}\right) \end{aligned}$$

Bousquet and Bottou '08

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$$\epsilon \sim O\left(\frac{1}{\sqrt{n}}\right)$$

$$n \sim O\left(\frac{1}{\epsilon^2}\right)$$

Strongly convex case

Method	Complexity
GD	$\mathcal{O}\left(1/\epsilon^2 \kappa \log\left(1/\epsilon\right)\right)$
SGD	$\mathcal{O}\left(1/\epsilon\right)$
SVRG	$\mathcal{O}\left(1/\epsilon^2 + \kappa\right) \log\left(1/\epsilon\right)\right)$
SARAH	$\mathcal{O}\left(1/\epsilon^2 + \kappa\right) \log\left(1/\epsilon\right)\right)$

Bousquet and Bottou '08

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Convex case

Method	Complexity
GD	$\mathcal{O}\left(1/\epsilon^3\right)$
SGD	$\mathcal{O}\left(1/\epsilon^2\right)$
SVRG	$\mathcal{O}\left(1/\epsilon^2\right))$
SARAH	$\mathcal{O}\left((1/\epsilon^2 + 1/\epsilon)\log(1/\epsilon)\right)$

Is stochastic gradient the best we can do? And what about nonconvex problems...?

To be continued by Frank Curtis

Optimization Methods for Supervised Machine Learning: From Linear Models to Deep Learning, Part II

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joint work with

Katya Scheinberg, Lehigh University

INFORMS Annual Meeting, Houston, TX, USA

23 October 2017

Outline

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Deep Neural Networks

Nonconvex Optimization

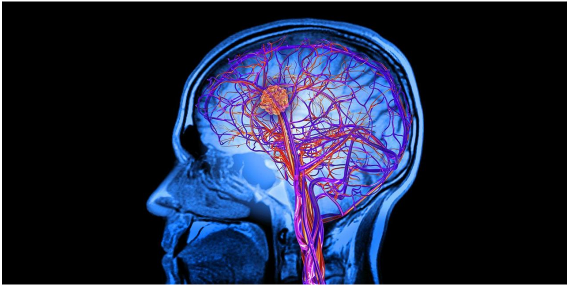
Second-Order Methods

Thanks

What is a neural network?

What is a neural network?

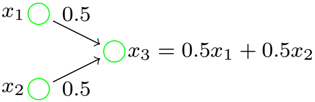
- A computer brain (artificial intelligence!)



http://www.bbc.com/future/tags/brain

What is a neural network?

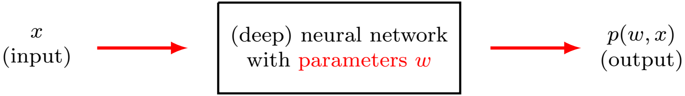
- A computer brain (artificial intelligence!)
- A computational graph
  - . . . defined using neuroscience jargon (e.g., node $\equiv$ neuron)



https://www.extremetech.com/extreme/151696-ibm-on-track-to-building-artificial-synapses

What is a neural network?

- A computer brain (artificial intelligence!)
- A computational graph
  - ...defined using neuroscience jargon (e.g., node ≡ neuron)
- A function! ...defined by some parameters



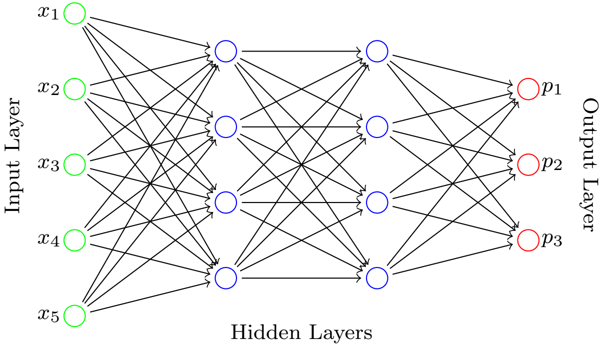
Learning

Neural networks do not learn on their own.

- In supervised learning, we train them by giving them inputs...
- ...and use optimization to better match their outputs to known outputs.
- (After, we hope they give the right outputs when they are unknown!)

We optimize the parameters ≡ weights ≡ decision variables.

Feed forward network, fully connected



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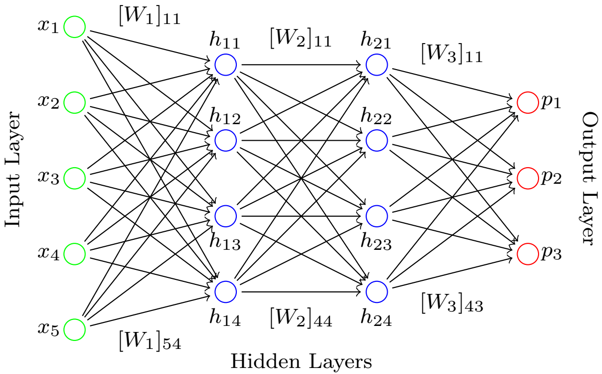

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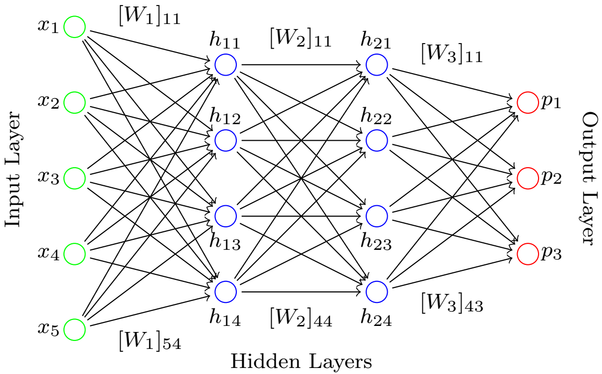
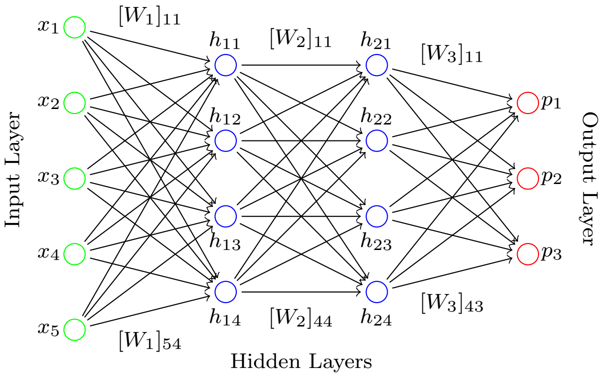


$$h_1 = s_1(W_1 x + \omega_1)$$

Feed forward network, fully connected



$$p(w, x) = s_3(W_3(s_2(W_2(s_1(W_1 x + \omega_1)) + \omega_2)) + \omega_3)$$

Training

As before, we have an optimization problem of the form

$$\min_{w \in \mathcal{W}} \mathbb{E}[\ell(p(w, x), y)]$$

or, with training data, of the form

$$\min_{w \in \mathcal{W}} \frac{1}{n} \sum_{i=1}^{n} \ell(p(w, x_i), y_i)$$

where

$$p(w, x) = s_3(W_3(s_2(W_2(s_1(W_1 x + \omega_1)) + \omega_2)) + \omega_3)$$

Example: Image classification

Humans can easily determine digits/letters from arrangements of pixels

Bottou et al., Optimization Methods for Large-Scale Machine Learning, *SIAM Review* (to appear)

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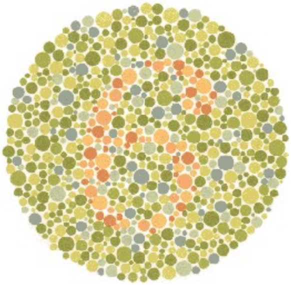

. . . for the most part.

(I'm told there's a number there!)

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https://colormax.org/color-blind-test/

Convolutional neural networks

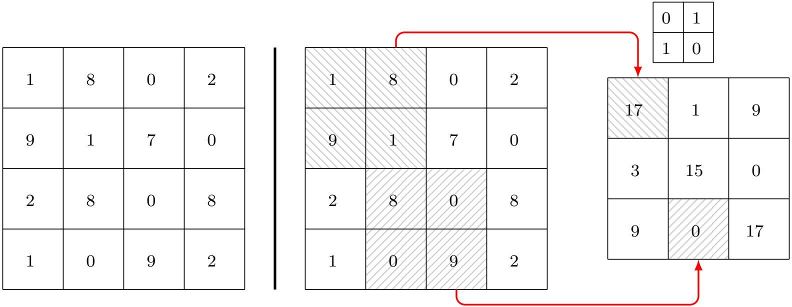
A modern tool for image classification is a convolutional neural network (CNN)

- These work by trying to capture spatial relationships between input values

Convolutional neural networks

A modern tool for image classification is a convolutional neural network (CNN)

- These work by trying to capture spatial relationships between input values
- For example, in the example below, a filter is applied—to compute the sum of elementwise products—to look for a diagonal pattern



- Here, the data is a matrix, but these can be translated to vector operations.

Anjelica Huston (not Houston!)

A random filter simply blurs the data, which doesn't help

https://www.filmcomment.com/article/interview-anjelica-huston

Anjelica Huston (not Houston!)

. . . but certain filters can reveal edges and other features

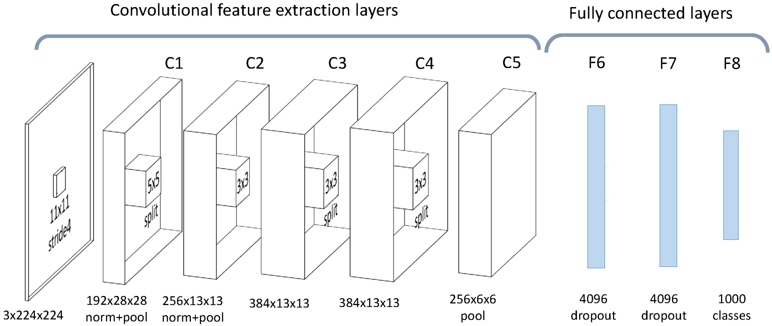
(There are plenty of Python tools for playing around like this.)

https://www.filmcomment.com/article/interview-anjelica-huston

Large-scale network

A full large-scale network involves various other components/tools:

- rectification, normalization, pooling, regularization, etc.

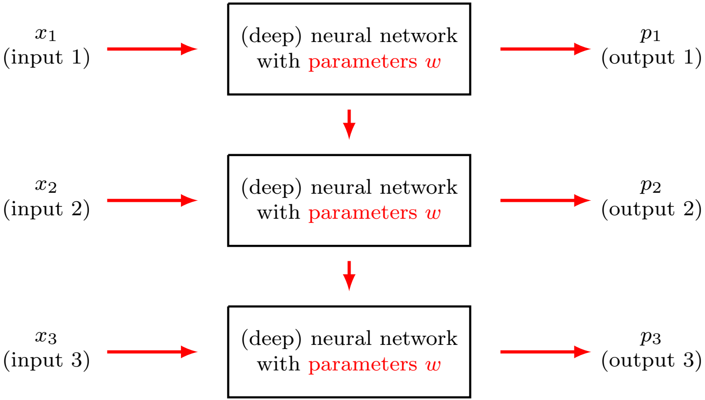


This network involves over 60 million parameters. Need good algorithms!

Bottou et al., Optimization Methods for Large-Scale Machine Learning, *SIAM Review* (to appear)

Recurrent neural networks

These try to capture temporal relationships between input values.



- Video classification, speech recognition, text classification, etc.

Outline

Deep Neural Networks

Nonconvex Optimization

Second-Order Methods

Thanks

Back propagation

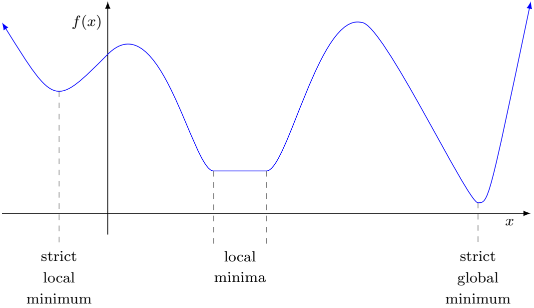
How do we optimize?

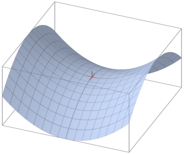
- Same as always!
- Compute derivatives, but how?
- Back propagation, i.e., automatic differentiation
- Then we need an optimization algorithm in which to use them.

Main challenges:

- "Full gradient" involves loop over all data, which is expensive
- . . . so consider stochastic methods, as previously mentioned.
- However, these problems are large-scale and nonconvex.

Global minima, local minima, saddle points, etc.





- These textbook illustrations might be misleading.
- The “landscape” of the objective function defined by a deep neural network is something of great interest these days.

https://upload.wikimedia.org/wikipedia/commons/4/40/Saddle_point.png

How to optimize?

It is not clear where a gradient-based method might converge.

- However, (stochastic) gradient-based methods seem to work well!
- They provably avoid saddle points with high probability.
- ... and often converge to "good" stationary points.

How to optimize?

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- However, (stochastic) gradient-based methods seem to work well!
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- . . . and often converge to "good" stationary points.

Open questions:

- How to characterize the behavior of different methods?
- How to characterize the generalization properties of solutions?
- What algorithms are the most effective at finding points with good generalization properties?

We will not answer these; instead, we'll simply describe/motivate some methods.

Outline

Deep Neural Networks

Nonconvex Optimization

Second-Order Methods

Thanks

First- versus second-order

First-order methods follow a steepest descent methodology:

$$w_{k+1} \leftarrow w_k - \alpha_k \nabla f(w_k)$$

Second-order methods follow Newton's methodology:

$$w_{k+1} \leftarrow w_k - \alpha_k [\nabla^2 f(w_k)]^{-1} \nabla f(w_k),$$

which one should view as minimizing a quadratic model of f at w_k:

$$f(w_k) + \nabla f(w_k)^T (w - w_k) + \tfrac{1}{2}(w - w_k)^T \nabla^2 f(w_k)(w - w_k)$$

First- versus quasi-second-order

First-order methods follow a steepest descent methodology:

$$w_{k+1} \leftarrow w_k - \alpha_k \nabla f(w_k)$$

Second-order methods follow Newton's methodology:

$$w_{k+1} \leftarrow w_k - \alpha_k M_k \nabla f(w_k),$$

which one should view as minimizing a quadratic model of f at w_k:

$$f(w_k) + \nabla f(w_k)^T (w - w_k) + \tfrac{1}{2}(w - w_k)^T H_k (w - w_k)$$

Might also replace the Hessian with an approximation H_k with inverse M_k

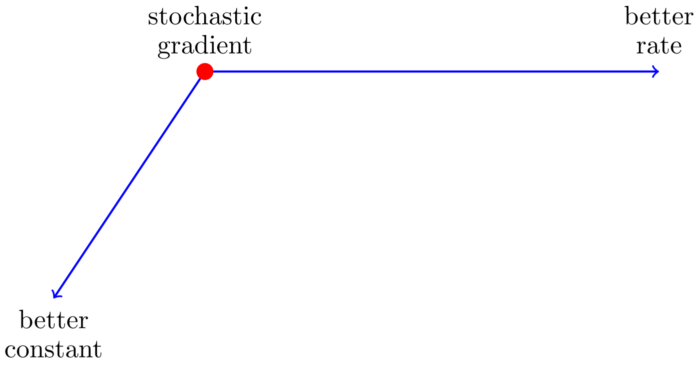
Why second-order?

Second-order methods are expensive!

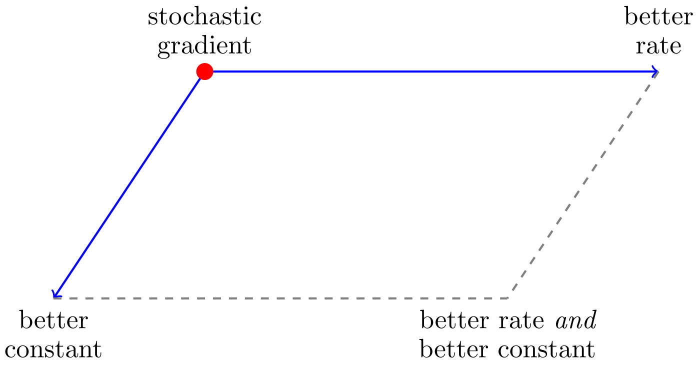
- Yes, but judicious use of second-order information can help
- . . . and the resulting methods can be made nearly as cheap as SG.

Overall, there are various ways to improve upon SG. . .

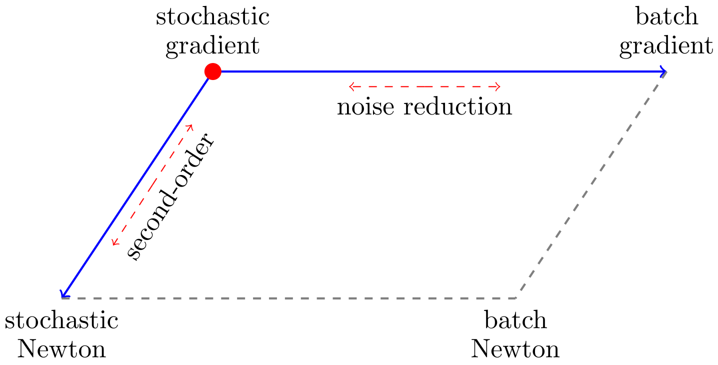
What can be improved?



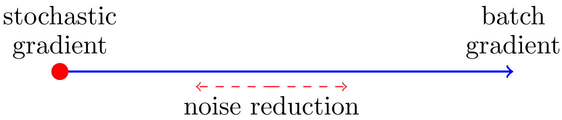
What can be improved?



Two-dimensional schematic of methods

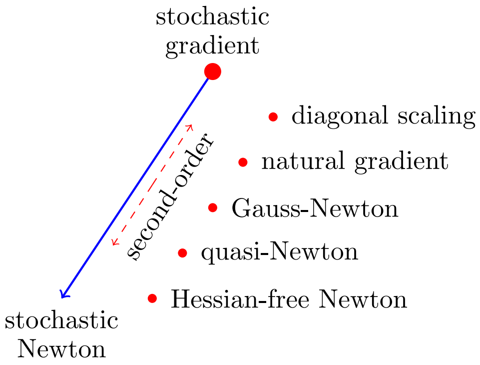


2D schematic: Noise reduction methods



- dynamic sampling
- gradient aggregation
- iterate averaging

2D schematic: Second-order methods



So, why second-order?

Traditional motivation: fast local convergence guarantees

- Hard to achieve in large-scale stochastic settings

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Recent motivation (last few years): better complexity properties

- Many are no better than first-order methods in terms of complexity
- ...and ones with better complexity aren't necessarily best in practice (yet)

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- Many are no better than first-order methods in terms of complexity
- ...and ones with better complexity aren't necessarily best in practice (yet)

Other reasons?

- Adaptive, natural scaling (gradient descent $\approx 1/L$ while Newton ≈ 1)
- Mitigate effects of ill-conditioning
- Easier to tune parameters(?)
- Better at avoiding saddle points(?)
- Better trade-off in parallel and distributed computing settings
- New algorithms! Not analyzing the same old

Framework #1: Matrix-free (Gauss-)Newton

Compute each step by applying an iterative method to solve

$$H_k s_k = -g_k$$

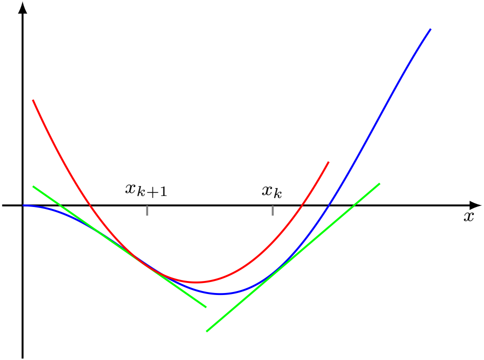
potentially with regularization, within a trust region, etc.

This can be computationally efficient since

- H_k can be defined by a subsample of data.
- Matrix-vector products can be computed without forming the matrix
- ... using similar principles as in back propagation.
- The linear system need not be solved exactly.

Quasi-Newton (deterministic setting)

Only *approximate* second-order information with gradient displacements:



Secant equation $H_k y_k = s_k$ to match gradient of f at w_k, where

$$s_k := w_{k+1} - w_k \quad \text{and} \quad y_k := \nabla f(w_{k+1}) - \nabla f(w_k)$$

Framework #2: Quasi-Newton

How can this idea be adapted to the stochastic setting?

- Idea #1: Replace y_k by displacement using the same sample, i.e.,

$$\nabla_{\mathcal{S}_k} f(w_{k+1}) - \nabla_{\mathcal{S}_k} f(w_k).$$

  (This doubles the number of stochastic gradients, but maybe worthwhile?)

- Idea #2: Replace y_k by action on a (subsampled) Hessian, i.e.,

$$\nabla^2_{\mathcal{S}_k^H} f(w_{k+1}) s_k$$

  (This requires matrix-vector products with a Hessian.)

- ...other ideas?

Outline

OptML @ Lehigh

Please visit the OptML @ Lehigh website!

- http://optml.lehigh.edu