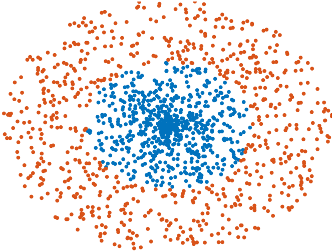
Single-Layer Neural Networks

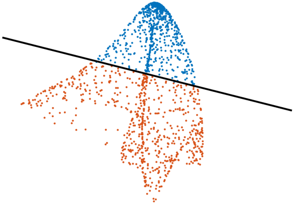
Numerical Methods for Deep Learning

Motivation: Nonlinear Models

In general, impossible to find a linear separator between classes



input features



transformed features

Goal/Trick
Embed the points in higher dimension and/or move the points to make them linearly separable

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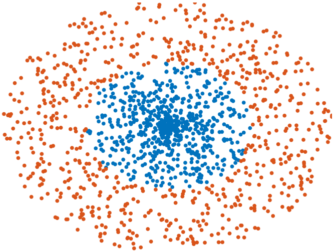

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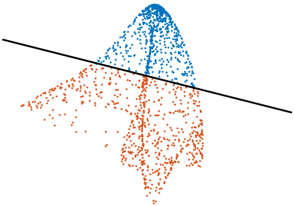


transformed features

Goal/Trick

Embed the points in higher dimension and/or move the points to make them linearly separable

Example: Linear Fitting

Assume $\mathbf{C} \in \mathbb{R}^{n_c \times n}$, $\mathbf{Y} \in \mathbb{R}^{n_f \times n}$ and $n \gg n_f$. Goal: Find $\mathbf{W} \in \mathbb{R}^{n_c \times n_f}$ such that

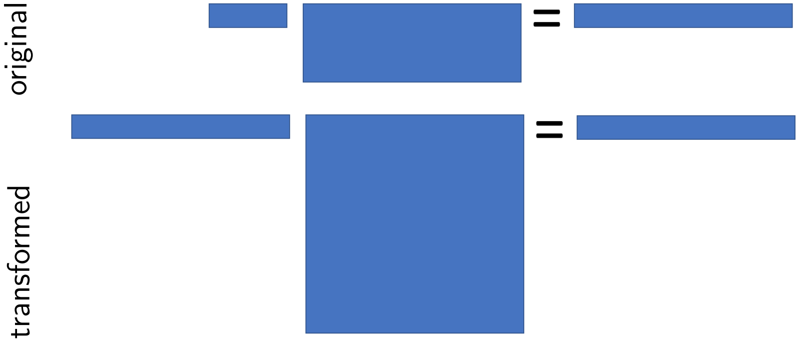
$$\mathbf{C} = \mathbf{W}\mathbf{Y}$$

If $\mathrm{rank}(\mathbf{Y}) < n$, there may be no solution.

Two options:

1. Regression: Solve $\min_{\mathbf{W}} \|\mathbf{W}\mathbf{Y} - \mathbf{C}\|_F^2 \rightsquigarrow$ always has solutions, but residual might be large
2. Nonlinear Model: Replace $\mathbf{Y}$ by $\sigma(\mathbf{K}\mathbf{Y})$ in regression, where σ is element-wise function (aka activation) and $\mathbf{K} \in \mathbb{R}^{m \times n_f}$ where $m \gg n_f$

Illustrating Nonlinear Models



Remarks

- instead of $\mathbf{WY} = \mathbf{C}$ solve $\hat{\mathbf{W}}\sigma(\mathbf{KY}) = \mathbf{C}$
- solve bigger problem $\leadsto$ memory, computation, ...
- what happens to $\mathrm{rank}(\sigma(\mathbf{KY}))$ when $\sigma(x) = x$?

Conjecture: Universal Approximation Properties

Given the data $\mathbf{Y} \in \mathbb{R}^{n_f \times n}$ and $\mathbf{C} \in \mathbb{R}^{n_c \times n}$ with $n \gg n_f$, there is nonlinear function $\sigma : \mathbb{R} \to \mathbb{R}$, a matrix $\mathbf{K} \in \mathbb{R}^{m \times n_f}$, and a bias $\mathbf{b} \in \mathbb{R}^m$ such that

$$\mathrm{rank}(\sigma(\mathbf{KY} + \mathbf{b})) = n.$$

Therefore, possible **??** to find $\mathbf{W} \in \mathbb{R}^{n_c \times m}$

$$\mathbf{W}\sigma(\mathbf{KY} + \mathbf{b}) = \mathbf{C}.$$

Choosing Nonlinear Model

$$\mathbf{W}\sigma(\mathbf{K}\mathbf{Y} + \mathbf{b}) = \mathbf{C}$$

- how to choose σ?
  - early days: motivated by neurons
  - popular choice: $\sigma(x) = \tanh(x)$ (smooth, bounded, ...)
  - nowadays: $\sigma(x) = \max(x, 0)$ (aka ReLU, rectified linear unit, non-differentiable, not bounded, simple)
- how to choose $\mathbf{K}$ and $\mathbf{b}$?
  - pick randomly $\rightsquigarrow$ branded as *extreme learning machines* **?**
  - train (optimize) $\rightsquigarrow$ done for most neural network
  - *deep learning* when neural network has many layers

First Experiment: Random Transformation

Select activation function and choose **K** and **b** randomly and solve the least-squares/classification problem

The Pros:

- universal approximation theorem: can interpolate any function
- very(!) easy to program
- can serve as a benchmark to more sophisticated methods

Some concerns:

- may require very large **K** (scale with n, number of examples)
- may not generalize well
- large dense linear algebra

`EELM_Peaks.m`

Learning the Weights

Assume that the number of examples, n, is very large.
Using random weights, $\mathbf{K}$ might need to be very large to fit training data.
Solution may not generalize well to test data.

Idea: Learn $\mathbf{K}$ and b from the data (in addition to $\mathbf{W}$)

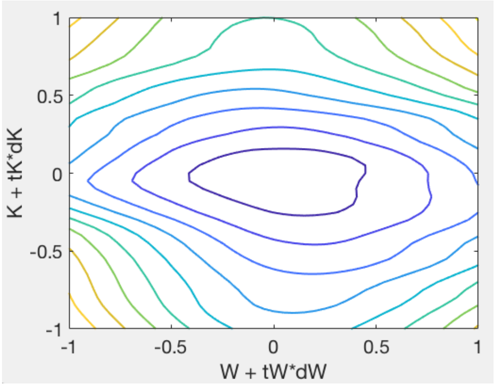
$$\min_{\mathbf{K},\mathbf{W},b} E(\mathbf{W}\sigma(\mathbf{K}\mathbf{Y} + \mathbf{b}), \mathbf{C}^{\text{obs}}) + \lambda R(\mathbf{W}, \mathbf{K}, \mathbf{b})$$

About this optimization problem:

- more unknowns $\mathbf{K} \in \mathbb{R}^{m \times n_f}$, $\mathbf{W} \in \mathbb{R}^{n_c \times m}$, $\mathbf{b} \in \mathbb{R}^m$
- non-convex problem $\rightsquigarrow$ local minima, careful initialization
- need to compute derivatives w.r.t. $\mathbf{K}, \mathbf{b}$

Non-Convexity

The optimization problem is non-convex. Simple illustration of cross-entropy along two random directions $d\mathbf{K}$ and $d\mathbf{W}$

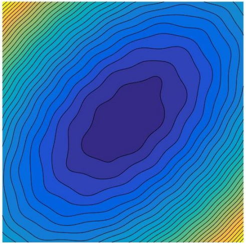


(see `ESingleLayer_PlotObjective.m`)

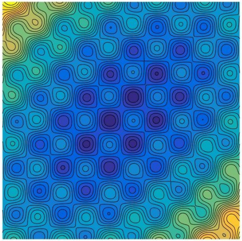
Expect worse when number of layers grows!

Training the Neural Network

- If non-convexity is not "too bad" can use standard gradient based methods
- If non-convexity is "ugly" need to modify standard methods (stochastic kick)
- If non-convexity is "bad" need global optimization techniques



good



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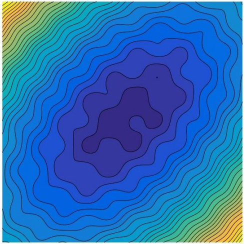

ugly

Recap: Differentiating Linear Algebra Expressions

Easy ones:

$$F_1(\mathbf{x}, \mathbf{y}) = \mathbf{x}^\top \mathbf{y} \qquad\qquad \mathbf{J}_\mathbf{x} F_1(\mathbf{x}, \mathbf{y}) = \mathbf{y}^\top$$
$$F_2(\mathbf{A}, \mathbf{x}) = \mathbf{A}\mathbf{x} \qquad\qquad \mathbf{J}_\mathbf{x} F_2(\mathbf{x}, \mathbf{y}) = \mathbf{A}$$

How about

$$F_3(\mathbf{A}, \mathbf{X}) = \mathbf{A}\mathbf{X} \qquad \mathbf{J}_{\mathrm{vec}(\mathbf{X})} F_3 = ???$$

Recall that

$$\mathrm{vec}(\mathbf{A}\mathbf{X}) = \mathrm{vec}(\mathbf{A}\mathbf{X}\mathbf{I}) = (\mathbf{I} \otimes \mathbf{A})\mathrm{vec}(\mathbf{X})$$

Therefore:

$$\mathbf{J}_{\mathrm{vec}(\mathbf{X})} F_3(\mathbf{A}, \mathbf{X}) = \mathbf{I} \otimes \mathbf{A}$$

Efficient mat-vec: $\mathbf{J}_{\mathrm{vec}(\mathbf{X})} F \mathbf{v} = \mathrm{vec}(\mathbf{A}\ \mathrm{mat}(\mathbf{v}))$

Training Single Layer Neural Network

Assume no regularization (easy to add) and re-write optimization problem as

$$\min_{\mathbf{W},\mathbf{K},b} E(\mathbf{C}^{\mathrm{obs}}, \mathbf{Z}, \mathbf{W}) \quad \text{with} \quad \mathbf{Z} = \sigma(\mathbf{K}\mathbf{Y} + b)$$

Agenda:

1. compute derivative of $\mathrm{vec}(\mathbf{Z})$ w.r.t. $\mathrm{vec}(\mathbf{K}), b$
2. use chain rule to get

$$\mathbf{J}_{\mathrm{vec}(\mathbf{K})}E = \mathbf{J}_{\mathrm{vec}(\mathbf{Z})}E(\mathbf{C}^{\mathrm{obs}}, \mathbf{Z}, \mathbf{W})\ \mathbf{J}_{\mathrm{vec}(\mathbf{K})}\mathbf{Z}$$
$$\mathbf{J}_{b}E = \mathbf{J}_{\mathrm{vec}(\mathbf{Z})}E(\mathbf{C}^{\mathrm{obs}}, \mathbf{Z}, \mathbf{W})\ \mathbf{J}_{b}\mathbf{Z}$$

3. efficient code for mat-vecs with $\mathbf{J}$ and $\mathbf{J}^\top$

Computing Jacobians

$$\mathbf{Z} = \sigma(\mathbf{K}\mathbf{Y} + b)$$

Recall that σ is applied element-wise.

$$\mathbf{J}_{\mathrm{vec}(\mathbf{K})}\mathbf{Z} = \mathrm{diag}(\sigma'(\mathbf{K}\mathbf{Y} + b))(\mathbf{Y}^\top \otimes \mathbf{I})$$

Efficient way to get matrix vector products

$$\begin{aligned}\mathbf{J}_{\mathrm{vec}(\mathbf{K})}\mathbf{Z}\mathbf{v} &= \mathrm{diag}(\sigma'(\mathbf{K}\mathbf{Y} + b))(\mathbf{Y}^\top \otimes \mathbf{I})\mathbf{v} \\ &= \mathrm{vec}\left(\sigma'(\mathbf{K}\mathbf{Y} + b) \odot (\mathrm{mat}(\mathbf{v})\mathbf{Y})\right)\end{aligned}$$

And for transpose get

$$\begin{aligned}(\mathbf{J}_{\mathrm{vec}(\mathbf{K})}\mathbf{Z})^\top\mathbf{u} &= (\mathbf{Y} \otimes \mathbf{I})\mathrm{diag}(\sigma'(\mathbf{K}\mathbf{Y} + b))\mathbf{u} \\ &= \mathrm{vec}\left(\sigma'(\mathbf{K}\mathbf{Y} + b) \odot \mathrm{mat}(\mathbf{u})\mathbf{Y}^\top\right)\end{aligned}$$

Class Problems: Derivatives of Single Layer

Derivations:

1. Compute $\mathbf{J}_b\mathbf{Z}v$ and $(\mathbf{J}_b\mathbf{Z})^\top\mathbf{u}$
2. Compute $\mathbf{J}_{\mathrm{vec}(\mathbf{Y})}\mathbf{Z}\mathbf{v}$ and $(\mathbf{J}_{\mathrm{vec}(\mathbf{Y})}\mathbf{Z})^\top\mathbf{u}$

Coding:

```
function[Z,JKt,Jbt,JYt,JK,Jb,JY] = singleLayer(K,b,Y)
% Returns Z = sigma(K*Y+b) and
%                         functions for J'*U and J*V
```

Testing:

1. Derivative check for Jacobian mat-vec
2. Adjoint tests for transpose, let $\mathbf{v}, \mathbf{u}$ be arbitray vectors

$$\mathbf{u}^\top\mathbf{J}\mathbf{v} \approx \mathbf{v}^\top\mathbf{J}^\top\mathbf{u}$$

Putting Things Together

Implement loss function of single-layer NN

$$E(\mathbf{K}, b, \mathbf{W}) \stackrel{def}{=} E(\mathbf{C}, \mathbf{Z}, \mathbf{W}), \quad \mathbf{Z} = \sigma(\mathbf{KY} + b)$$

```
function [Ec,dE] = singleLayerNNObjFun(x,Y,C,m)
% where x = [K(:); b; W(:)]
% evaluates single layer and computes cross entropy
%        and gradient (extend for approx. Hessian)
```

Use

1. $\nabla_{\mathbf{Z}} E = \mathbf{W}^\top \nabla_{\mathbf{S}} E(\mathbf{S}), \quad \mathbf{S} = \mathbf{WZ}$
2. $\nabla_{\mathbf{K}} E = \mathbf{J}_{\mathbf{K}}^\top \nabla_{\mathbf{Z}} E$
3. $\nabla_{\mathbf{b}} E = \mathbf{J}_{\mathbf{b}}^\top \nabla_{\mathbf{Z}} E$
4. $\nabla_{\mathbf{W}} E = \nabla_{\mathbf{S}} E(\mathbf{S}) \mathbf{Y}$

Test Problem

Before going to real data, let us try the *inverse crime*.
Generate data

```
n  = 500; nf = 50; nc = 10; m  = 40;
Wtrue = randn(nc,m);
Ktrue = randn(m,nf);
btrue = .1;

Y     = randn(nf,n);
Cobs  = exp(Wtrue*singleLayer(Ktrue,btrue,Y));
Cobs  = Cobs./sum(Cobs,1);
```

Goal: Reconstruct `Wtrue`, `Ktrue`, `btrue`!

Gauss-Newton Method

Goal: Use curvature information for fast convergence

$$\nabla_{\mathbf{K}} E(\mathbf{K}, \mathbf{b}, \mathbf{W}) = (\mathbf{J}_{\mathbf{K}}\mathbf{Z})^\top \nabla_{\mathbf{Z}} E(\mathbf{W}\sigma(\mathbf{K}\mathbf{Y} + \mathbf{b}), \mathbf{C}),$$

where $\mathbf{J}_{\mathbf{K}}\mathbf{Z} = \nabla_{\mathbf{K}}\sigma(\mathbf{K}\mathbf{Y} + \mathbf{b})^\top$.This means that Hessian is

$$\begin{aligned}\nabla^2_{\mathbf{K}} E(\mathbf{K}) &= (\mathbf{J}_{\mathbf{K}}\mathbf{Z})^\top \nabla^2_{\mathbf{Z}} E(\mathbf{C}, \mathbf{Z}, \mathbf{W}) \mathbf{J}_{\mathbf{K}}\mathbf{Z} \\ &\quad + \sum_{i=1}^{n} \sum_{j=1}^{m} \nabla^2_{\mathbf{K}} \sigma(\mathbf{K}\mathbf{Y} + \mathbf{b})_{ij} \nabla_{\mathbf{Z}} E(\mathbf{C}, \mathbf{Z}, \mathbf{W})_{ij}\end{aligned}$$

First term is spsd and we can compute it.
We neglect second term since

- can be indefinite and difficult to compute
- small if transformation is roughly linear or close to solution (easy to see for least-squares)

do the same for **b** and use full Hessian for **W** $\rightsquigarrow$ ignore coupling!

Experiment: Adversarial Example

Suppose you have trained your network $\rightsquigarrow \mathbf{K}, b, \mathbf{W}$ so that validation loss is low. This means that for most examples $\mathbf{y}$,

$$\mathbf{W}\sigma(\mathbf{K}\mathbf{y} + b) \approx \mathbf{c}.$$

An adversary might try to fool this classifier by adding a small perturbation $\mathbf{d}$ to the example to achieve a desired label $\hat{\mathbf{c}}$.

Formulate as optimization problem

$$\min_{\mathbf{d}} E(\mathbf{W}\sigma(\mathbf{K}(\mathbf{y} + \mathbf{d}) + b), \hat{\mathbf{c}})$$

- setup objective function
- think about constraints, regularization