Failures of Gradient-Based Deep Learning

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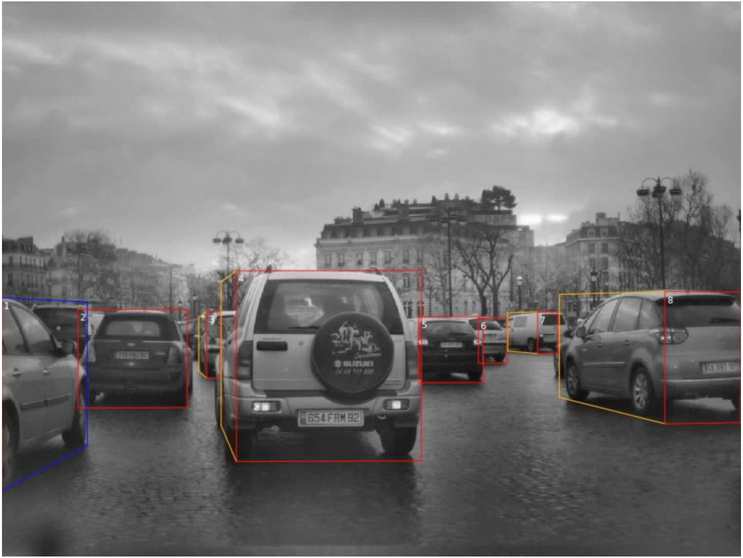
Deep Learning is Amazing ...



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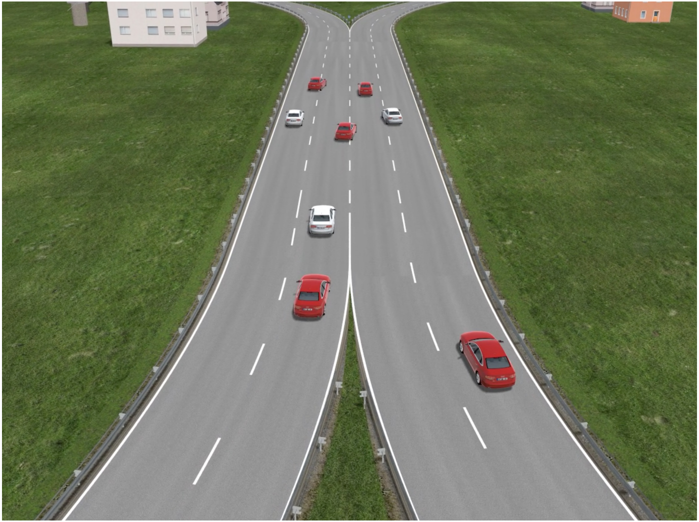

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INTEL IS BUYING MOBILEYE FOR $15.3 BILLION IN BIGGEST ISRAELI HI-TECH DEAL EVER

This Talk

Simple problems where standard deep learning either

- Does not work well
  - Requires prior knowledge for better architectural/algorithmic choices
  - Requires other than gradient update rule
  - Requiers to decompose the problem and add more supervision
- Does not work at all
  - No “local-search” algorithm can work
  - Even for “nice” distributions and well-specified models
  - Even with over-parameterization (a.k.a. improper learning)

Mix of theory and experiments

Outline

Piecewise-linear Curves: Motivation

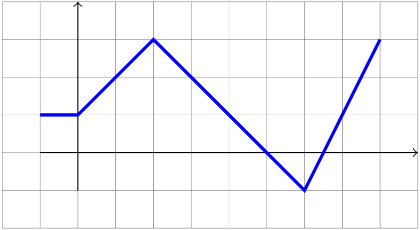
Piecewise-linear Curves

Problem: Train a piecewise-linear curve detector

Input: $\mathbf{f} = (f(0), f(1), \ldots, f(n-1))$ where

$$f(x) = \sum_{r=1}^{k} a_r [x - \theta_r]_+ \quad , \quad \theta_r \in \{0, \ldots, n-1\}$$

Output: Curve parameters $\{a_r, \theta_r\}_{r=1}^{k}$



First try: Deep AutoEncoder

- Encoding network, E_{w_1}: Dense(500,relu)-Dense(100,relu)-Dense($2k$)
- Decoding network, D_{w_2}: Dense(100,relu)-Dense(100,relu)-Dense(n)
- Squared Loss: $(D_{w_2}(E_{w_1}(\mathbf{f})) - \mathbf{f})^2$

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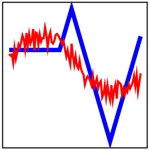
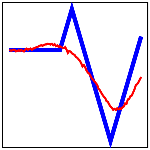
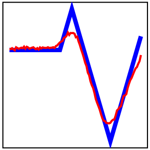
- Doesn't work well ...



500 iterations



10,000 iterations



50,000 iterations

Second try: Pose as a Convex Objective

Problem: Train a piecewise-linear curve detector

Input: $\mathbf{f} \in \mathbb{R}^n$ where $f(x) = \sum_{r=1}^{k} a_r [x - \theta_r]_+$
Output: Curve parameters $\{a_r, \theta_r\}_{r=1}^{k}$

Convex Formulation

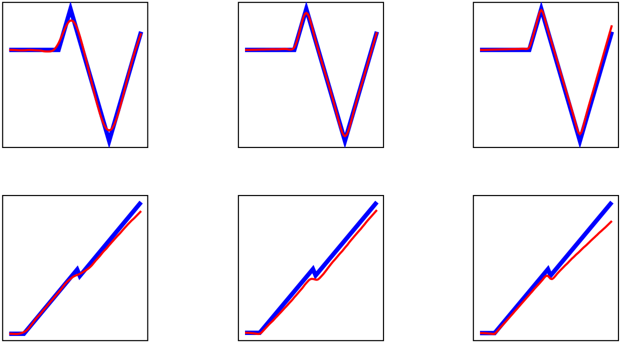
- Let $\mathbf{p} \in \mathbb{R}^{n,n}$ be a k-sparse vector whose k max/argmax elements are $\{a_r, \theta_r\}_{r=1}^{k}$
- Observe: $\mathbf{f} = W\mathbf{p}$ where $W \in \mathbb{R}^{n,n}$ is s.t. $W_{i,j} = [i - j + 1]_+$
- Learning approach — linear regression: Train a one-layer fully connected network on $(\mathbf{f}, \mathbf{p})$ examples:

$$\min_{U} \mathbb{E}\left[(U\mathbf{f} - \mathbf{p})^2\right] = \mathbb{E}\left[(U\mathbf{f} - W^{-1}\mathbf{f})^2\right]$$

Second try: Pose as a Convex Objective

$$\min_U \mathbb{E}\left[(U\mathbf{f}-\mathbf{p})^2\right] = \mathbb{E}\left[(U\mathbf{f}-W^{-1}\mathbf{f})^2\right]$$

- Convex; Realizable; but still doesn't work well ...



500 iterations 10,000 iterations 50,000 iterations

What went wrong?

Theorem

The convergence of SGD is governed by the condition number of $W^\top W$*, which is large:*

$$\frac{\lambda_{\max}(W^\top W)}{\lambda_{\min}(W^\top W)} = \Omega(n^{3.5})$$

$\Rightarrow$ *SGD requires* $\Omega(n^{3.5})$ *iterations to reach* U *s.t.* $\left\|\mathbb{E}[U] - W^{-1}\right\| < 1/2$

- Note: Adagrad/Adam doesn't work because they perform diagonal conditioning

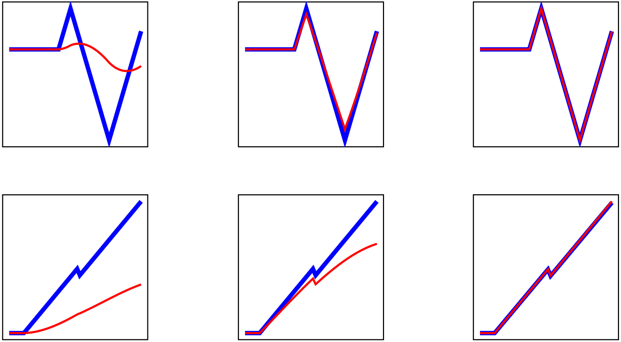
3rd Try: Pose as a Convolution

- $\mathbf{p} = W^{-1}\mathbf{f}$
- Observation:

$$W^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ -2 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & -2 & 1 & \cdots \\ 0 & 0 & 1 & -2 & \cdots \\ \vdots & \vdots & \vdots & & \end{pmatrix}$$

- $W^{-1}\mathbf{f}$ is 1D convolution of $\mathbf{f}$ with "2nd derivative" filter $(1, -2, 1)$
- Can train a one-layer convnet to learn filter (problem in $\mathbb{R}^3$!)

Better, but still doesn't work well ...



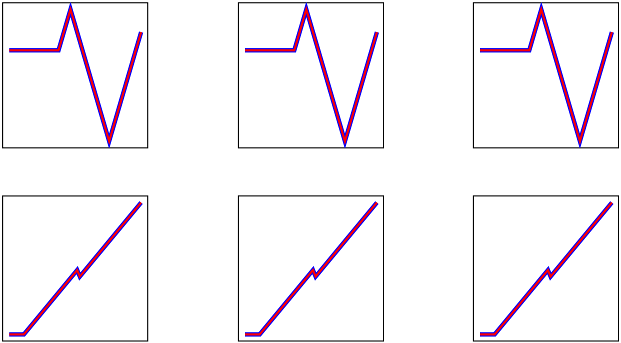
500 iterations 10,000 iterations 50,000 iterations

- Theorem: Condition number reduced to $\Theta(n^3)$. Convolutions aid geometry!
- But, $\Theta(n^3)$ is very disappointing for a problem in $\mathbb{R}^3$ ...

4th Try: Convolution + Preconditioning

- ConvNet is equivalent to solving $\min_{\mathbf{x}} \mathbb{E}\left[(F\mathbf{x}-\mathbf{p})^2\right]$ where F is $n \times 3$ matrix with $(f(i-1), f(i), f(i+1))$ at row i
- Observation: Problem is now low-dimensional, so can easily precondition
  - Compute empirical approximation C of $\mathbb{E}[F^\top F]$
  - Solve $\min_{\mathbf{x}} \mathbb{E}[(FC^{-1/2}\mathbf{x}-\mathbf{p})^2]$
  - Return $C^{1/2}\mathbf{x}$
- Condition number of $FC^{-1/2}$ is close to 1

Finally, it works ...



500 iterations | 10,000 iterations | 50,000 iterations

Remark:

- Use of convnet allows for efficient preconditioning
- Estimating and manipulating 3×3 rather than $n \times n$ matrices.

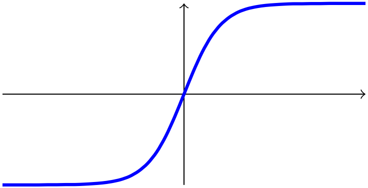
Lesson Learned

- SGD might be extremely slow
- Prior knowledge allows us to:
  - Choose a better architecture (not for expressivity, but for a better geometry)
  - Choose a better algorithm (preconditioned SGD)

Outline

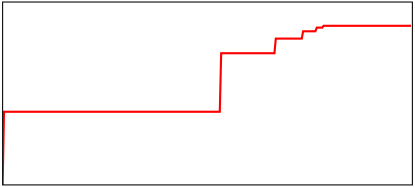
Flat Activations

Vanishing gradients due to saturating activations (e.g. in RNN's)



Flat Activations

Problem: Learning $\mathbf{x} \mapsto u(\langle \mathbf{w}^\star, \mathbf{x} \rangle)$ where u is a fixed step function



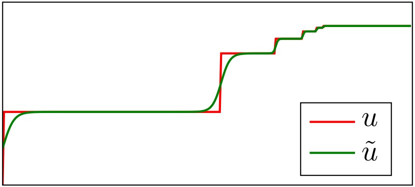
Optimization problem:

$$\min_{\mathbf{w}} \mathop{\mathbb{E}}_{\mathbf{x}}[(u(N_{\mathbf{w}}(\mathbf{x})) - u(\mathbf{w}^{\star\top}\mathbf{x}))^2]$$

$u'(z) = 0$ almost everywhere $\rightarrow$ can't apply gradient-based methods

Flat Activations: Smooth approximation

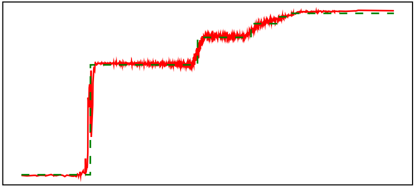
Smooth approximation: replace u with $\tilde{u}$ (similar to using sigmoids as gates in LSTM's)



Sometimes works, but slow and only approximate result. Often completely fails

Approach: End-to-end

$$\min_{\mathbf{w}} \mathbb{E}_{\mathbf{x}}[(N_{\mathbf{w}}(\mathbf{x}) - u(\mathbf{w}^{\star\top}\mathbf{x}))^2]$$



(3 ReLU + 1 linear layers; 10000 iterations)

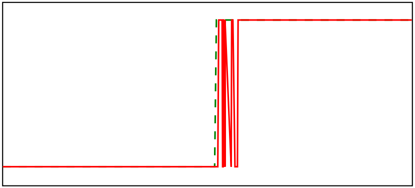
Slow train+test time; curve not captured well

Flat Activations: Multiclass

Approach: Multiclass

$$\min_{\mathbf{w}} \mathbb{E}_{\mathbf{x}}[\ell(N_{\mathbf{w}}(\mathbf{x}), y(\mathbf{x}))]$$

$N_{\mathbf{w}}(\mathbf{x})$: to which step does $\mathbf{x}$ belong



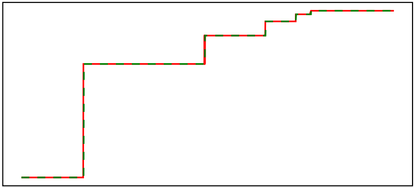
Problem capturing boundaries

Flat Activations: "Forward only" backpropagation

Different approach (Kalai & Sastry 2009, Kakade, Kalai, Kanade, Shamir 2011): Gradient descent, but replace gradient with something else

- Objective: $\min_{\mathbf{w}} \mathbb{E}_{\mathbf{x}} \left[\frac{1}{2} \left((u(\mathbf{w}^\top \mathbf{x})) - u(\mathbf{w}^{\star\top} \mathbf{x}) \right)^2 \right]$
- Gradient: $\nabla = \mathbb{E}_{\mathbf{x}} \left[\left(u(\mathbf{w}^\top \mathbf{x}) - u(\mathbf{w}^{\star\top} \mathbf{x}) \right) \cdot u'(\mathbf{w}^\top \mathbf{x}) \cdot \mathbf{x} \right]$
- Non-gradient direction: $\tilde{\nabla} = \mathbb{E}_{\mathbf{x}} \left[(u(\mathbf{w}^\top \mathbf{x}) - u(\mathbf{w}^{\star\top} \mathbf{x}))\mathbf{x} \right]$
- Interpretation: "Forward only" backpropagation

Flat Activation



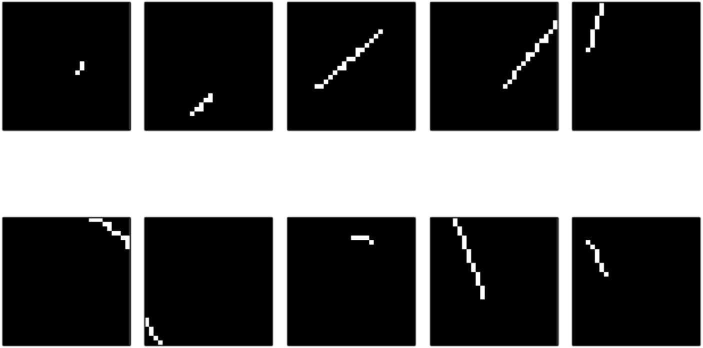
(linear; 5000 iterations)

- Best results, and smallest train+test time
- Analysis (KS09, KKKS11): Needs $\mathcal{O}(L^2/\epsilon^2)$ iterations if u is L-Lipschitz
- Lesson learned: Local search works, but not with the gradient ...

Outline

End-to-End vs. Decomposition

- Input $\mathbf{x}$: k-tuple of images of random lines
- $f_1(\mathbf{x})$: For each image, whether slope is negative/positive
- $f_2(\mathbf{x})$: return parity of slope signs
- Goal: Learn $f_2(f_1(\mathbf{x}))$



End-to-End vs. Decomposition

- Architecture: Concatenation of Lenet and 2-layer ReLU, linked by sigmoid
- End-to-end approach: Train overall network on primary objective
- Decomposition approach: Augment objective with loss specific to first net, using per-image labels

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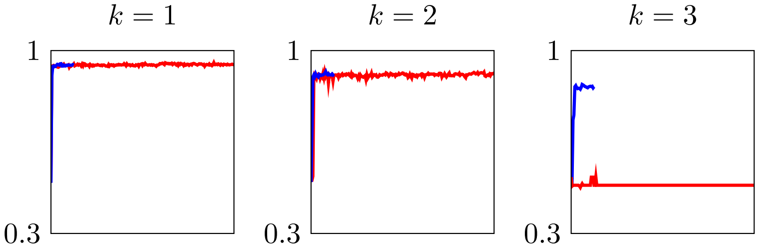


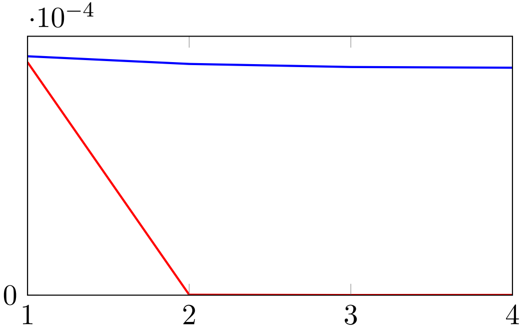
20000 iterations

End-to-End vs. Decomposition

- Why end-to-end training doesn't work ?
  - Similar experiment by Gulcehre and Bengio, 2016
  - They suggest "local minima" problems
  - We show that the problem is different

End-to-End vs. Decomposition

- Why end-to-end training doesn't work ?
  - Similar experiment by Gulcehre and Bengio, 2016
  - They suggest "local minima" problems
  - We show that the problem is different
- Signal-to-Noise Ratio (SNR) for random initialization:
  - End-to-end (red) vs. decomposition (blue), as a function of k
  - SNR of end-to-end for $k \geq 3$ is below the precision of float32



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Learning Many Orthogonal Functions

- Let $\mathcal{H}$ be a hypothesis class of orthonormal functions: $\forall h, h' \in \mathcal{H}$, $\mathbb{E}[h(\mathbf{x})h'(\mathbf{x})] = 0$

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- (Improper) learning of $\mathcal{H}$ using gradient-based deep learning:
  - Learn the parameter vector, $\mathbf{w}$, of some architecture, $p_{\mathbf{w}} : X \to \mathbb{R}$
  - For every target $h \in \mathcal{H}$, the learning task is to solve:

$$\min_{\mathbf{w}} F_h(\mathbf{w}) := \mathbb{E}_{\mathbf{x}}[\ell(p_{\mathbf{w}}(\mathbf{x}), h(\mathbf{x})]$$

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  - Start with a random $\mathbf{w}$ and update the weights based on $\nabla F_h(\mathbf{w})$
- Analysis tool: How much $\nabla F_h(\mathbf{w})$ tells us about the identity of h ?

Analysis: how much information in the gradient?

$$\min_{\mathbf{w}} F_h(\mathbf{w}) := \mathop{\mathbb{E}}_{\mathbf{x}}[\ell(p_{\mathbf{w}}(\mathbf{x}), h(\mathbf{x})]$$

- Theorem: For every $\mathbf{w}$, there are many pairs $h, h' \in \mathcal{H}$ s.t. $\mathbb{E}_{\mathbf{x}}[h(\mathbf{x})h'(\mathbf{x})] = 0$ while

$$\|\nabla F_h(\mathbf{w}) - \nabla F_{h'}(\mathbf{w})\|^2 = O\left(\frac{1}{|\mathcal{H}|}\right)$$

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- Proof idea: show that if the functions in $\mathcal{H}$ are orthonormal then, for every $\mathbf{w}$,

$$\mathrm{Var}(\mathcal{H}, F, \mathbf{w}) := \mathbb{E}_h \left\|\nabla F_h(\mathbf{w}) - \mathbb{E}_{h'} \nabla F_{h'}(\mathbf{w})\right\|^2 = O\left(\frac{1}{|\mathcal{H}|}\right)$$

- To do so, express every coordinate of $\nabla p_{\mathbf{w}}(\mathbf{x})$ using the orthonormal functions in $\mathcal{H}$

Proof idea

Assume the squared loss, then

$$\begin{aligned}\nabla F_h(\mathbf{w}) &= \mathop{\mathbb{E}}_{\mathbf{x}}[(p_{\mathbf{w}}(\mathbf{x}) - h(\mathbf{x})\,\nabla p_{\mathbf{w}}(\mathbf{x})] \\ &= \underbrace{\mathop{\mathbb{E}}_{\mathbf{x}}[p_{\mathbf{w}}(\mathbf{x})\,\nabla p_{\mathbf{w}}(\mathbf{x})]}_{\text{independent of } h} - \mathop{\mathbb{E}}_{\mathbf{x}}[h(\mathbf{x})\,\nabla p_{\mathbf{w}}(\mathbf{x})]\end{aligned}$$

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$$= \underbrace{\mathbb{E}_{\mathbf{x}}[p_{\mathbf{w}}(\mathbf{x})\,\nabla p_{\mathbf{w}}(\mathbf{x})]}_{\text{independent of } h} - \mathbb{E}_{\mathbf{x}}[h(\mathbf{x})\,\nabla p_{\mathbf{w}}(\mathbf{x})]$$

- Fix some j and denote $g(\mathbf{x}) = \nabla_j p_{\mathbf{w}}(\mathbf{x})$
- Can expand $g = \sum_{i=1}^{|\mathcal{H}|} \langle h_i, g\rangle h_i + \text{orthogonal component}$
- Therefore, $\mathbb{E}_h\left(\mathbb{E}_{\mathbf{x}}[h(\mathbf{x})\,g(\mathbf{x})]\right)^2 \leq \frac{\mathbb{E}_{\mathbf{x}}[g(\mathbf{x})^2]}{|\mathcal{H}|}$
- It follows that

$$\mathrm{Var}(\mathcal{H}, F, \mathbf{w}) \;\leq\; \frac{\mathbb{E}_{\mathbf{x}}[\|\nabla p_{\mathbf{w}}(\mathbf{x})\|^2]}{|\mathcal{H}|}$$

Example: Parity Functions

- $\mathcal{H}$ is the class of parity functions over $\{0,1\}^d$ and $\mathbf{x}$ is uniformly distributed
- There are 2^d orthonormal functions, hence there are many pairs $h, h' \in \mathcal{H}$ s.t. $\mathbb{E}_{\mathbf{x}}[h(\mathbf{x})h'(\mathbf{x})] = 0$ while $\|\nabla F_h(\mathbf{w}) - \nabla F_{h'}(\mathbf{w})\|^2 = O(2^{-d})$

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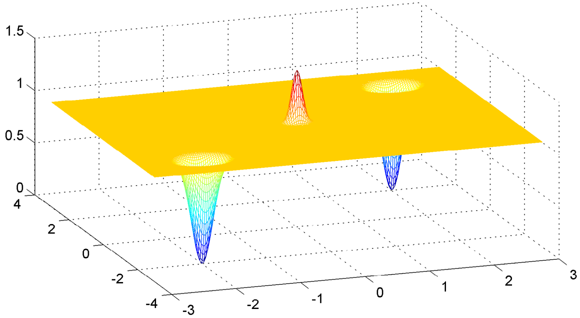
Remark:

- Similar hardness result can be shown by combining existing results:
  - Parities on uniform distribution over $\{0,1\}^d$ is difficult for statistical query algorithms (Kearns, 1999)
  - Gradient descent with approximate gradients can be implemented with statistical queries (Feldman, Guzman, Vempala 2015)

Visual Illustration: Linear-Periodic Functions

$F_h(\mathbf{w}) = \mathbb{E}_{\mathbf{x}}[(\cos(\mathbf{w}^\top \mathbf{x}) - h(\mathbf{x}))^2]$ for $h(\mathbf{x}) = \cos([2,2]^\top \mathbf{x})$, in 2 dimensions, $\mathbf{x} \sim \mathcal{N}(0, I)$:



- No local minima/saddle points
- However, extremely flat unless very close to optimum
  $\Rightarrow$ difficult for gradient methods, especially stochastic
- In fact, difficult for any local-search method

Summary

- Cause of failures: optimization can be difficult for geometric reasons other than local minima / saddle points
  - Condition number, flatness
  - Using bigger/deeper networks doesn't always help
- Remedies: prior knowledge can still be important
  - Convolution can improve geometry (and not just sample complexity)
  - "Other than gradient" update rule
  - Decomposing the problem and adding supervision can improve geometry
- Understanding the limitations: While deep learning is great, understanding the limitations may lead to better algorithms and/or better theoretical guarantees
- For more information:
  - "Failures of Deep Learning": arxiv 1703.07950
  - `github.com/shakedshammah/failures_of_DL`