[DLT 3-4]
Optimization and generalization of deep networks: a *highly biased* margin perspective

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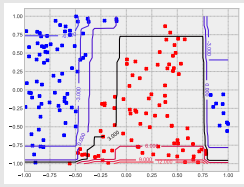
(with help from many friends!)

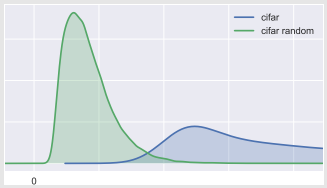
(Thanks for inviting me to Russia!)

Scope of these 4 lectures:

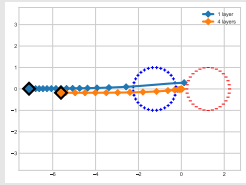
- 1-2: approximation theory.
- 3-4: margin perspective on optimization and generalization.
  This part is highly biased!



Margins.



Generalization.



Optimization.

Margins?

Margins?

- Margins are an existing theory for generalization/optimization;
  we can apply this theory to deep learning.
- There are other ways to study optimization generalization.
- As compared with yesterday, today will be **highly biased**, and include much work I am involved with.

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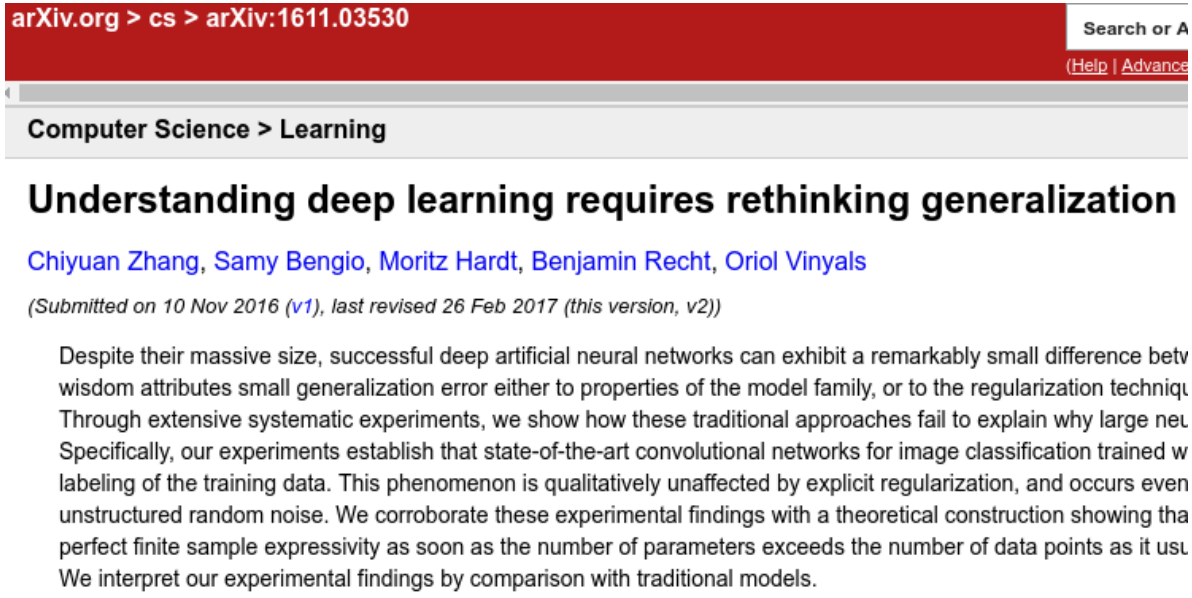

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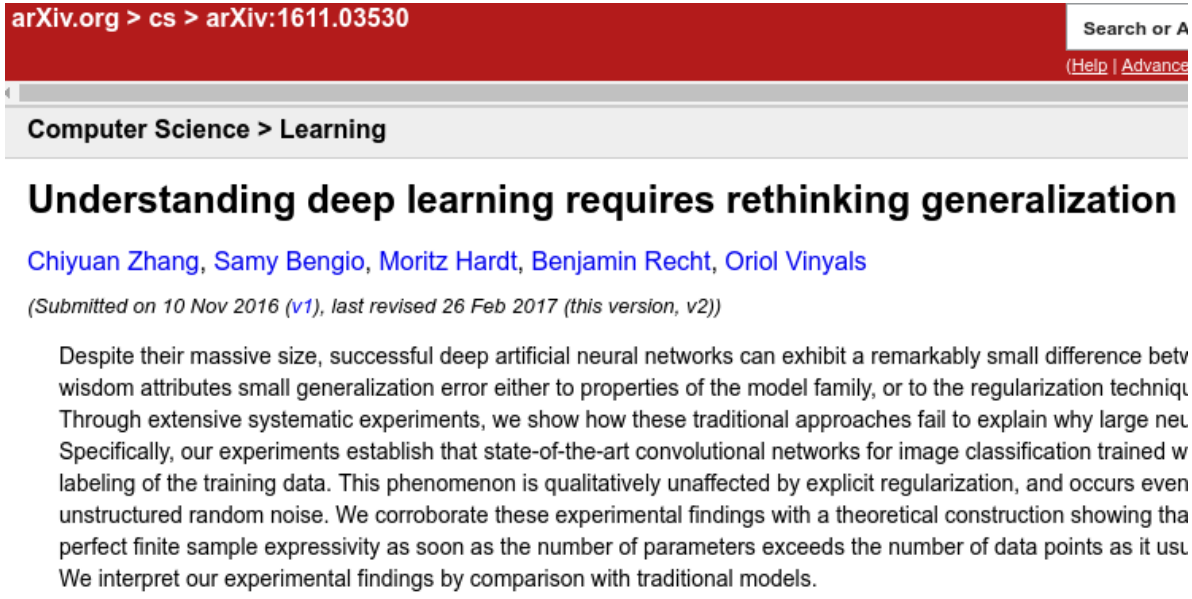

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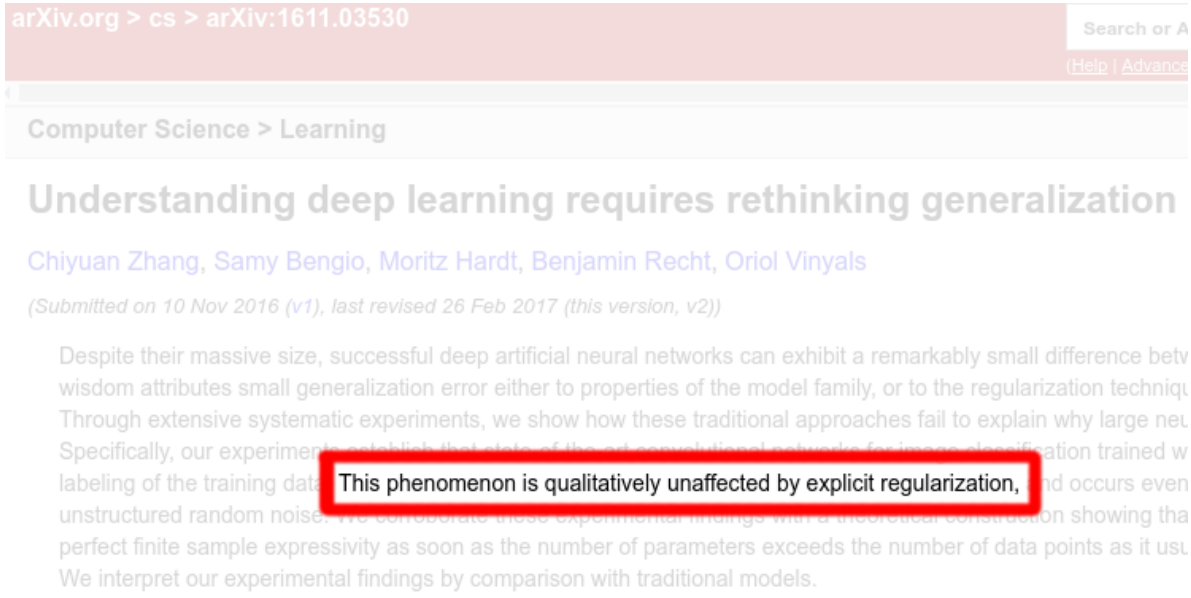

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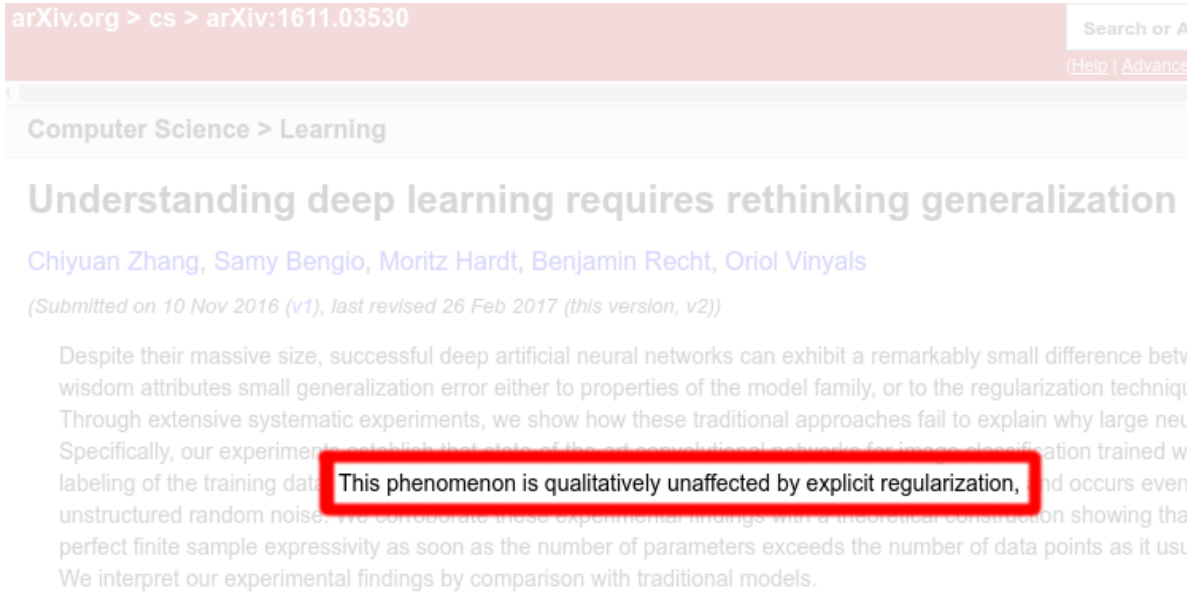

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- Wow! *Always* get 0 training error. (Even random labels!)
- Still generalizes.
- **Explicit regularization not needed;**
  sounds like boosting and margin theory!
- **Remark:** there are other ways to reason about this puzzle!

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Standard classifiers discretize real-valued predictions:

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History:

- Margins & optimization: Novikoff '62.
- Margins & generalization: Bartlett '96
  "For valid generalization the size of the weights is more important than the size of the network".
- Margins prominently used as an explanation of boosting.

Margins, boosting, and deep networks.

- Standard boosting methods can guarantee 0 training error.
  (Empirically observed with deep networks!)
- Standard boosting methods select large margin predictors.
  (Is this empirically observed with deep networks? Can we prove/disprove it?)
- Boosting methods have margin-based generalization bounds.
  (How about deep networks?)

Boosting overview.

- Greedily select classifiers $(h_i)_{i=1}^t$ and weights $w \in \mathbb{R}^t$ and output predictor $f_t(x) := \sum_j w_j h_j(x)$.
- Define margin $\min_i \frac{y_i f_t(x_i)}{\sum_j |w_j|}$.
- **Remarks.**
  - Standard method is **coordinate descent** on some risk; *not explicitly maximizing margins.*
  - $\sum_j |w_j| = \|w\|_1$ is due to coordinate descent; can prove theorems with this choice.

Large margin boosted classifiers generalize.

Theorem (Schapire-Freund-Bartlett-Lee, 1998).
Fix classifiers $\mathcal{H}$ with VC dimension $\text{VC}(\mathcal{H})$.
Given margin γ, with probability $\geq 1 - \delta$ over data $((x_i, y_i))^n$,
for any weights $w \in \mathbb{R}^t$ over $h_1, \ldots, h_t \in \mathcal{H}$,

$$\Pr[\text{error}] \leq \widehat{\Pr}[\gamma \text{ margin violation}] + \mathcal{O}\left(\frac{1}{\gamma}\sqrt{\frac{\text{VC}(\mathcal{H})\ln(n) + \ln(1/\delta)}{n}}\right).$$

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- Interpretation: treating $\|w\|_1$ as "complexity"
  ($\|w\|_1$ arises in $\widehat{\Pr}\left[\gamma > {}^{Yf_w(X)}/_{\|w\|_1}\right]$),
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- With random data, $\|w\|_1$ will be large and kill the bound.
- It is okay if $|\mathcal{H}| = \infty$!
- Story seems consistent with deep networks:
  can have big boosted classifier (big network),
  zero training error, and still generalize (if not random!).

Boosting methods find large margin boosted classifiers.

Theorem (T '13).
Let $\bar{\gamma}$ denote the maximum possible margin.
After $8\ln(n)/\bar{\gamma}^2$ iterations,
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- **Proof.** Adaboost uses exponential loss;
  thus $\ln \sum$ loss is like unnormalized minimum margin.
  Can then directly show it grows at least like $\bar{\gamma}\|w\|_1$.
- Together with previous slide, get low test error for boosting.
- A long history!
  - Novikoff '62: perceptron convergence rate via margins.
  - Schapire-Freund-Bartlett-Lee '98: asymptotic convergence to $\gamma/2$ margins (largest posible).
  - Zhang-Yu '05: more careful step sizes gives margin maximization.

Margin plots

Given $((x_i, y_i))_{i=1}^n$ and $f : \mathbb{R}^d \to \mathbb{R}^k$, plot CDF of

$$(x_i, y_i) \mapsto \frac{f(x_i) y_i}{C_f}.$$

This captures margins of whole training set.

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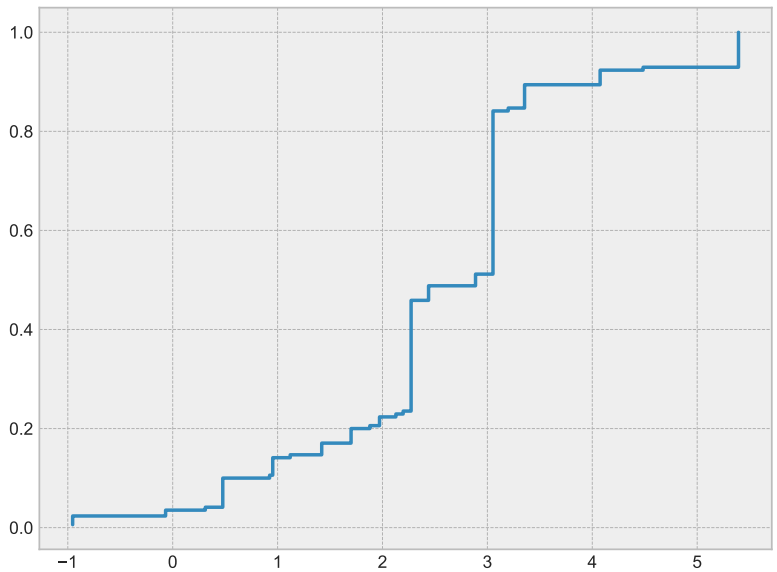
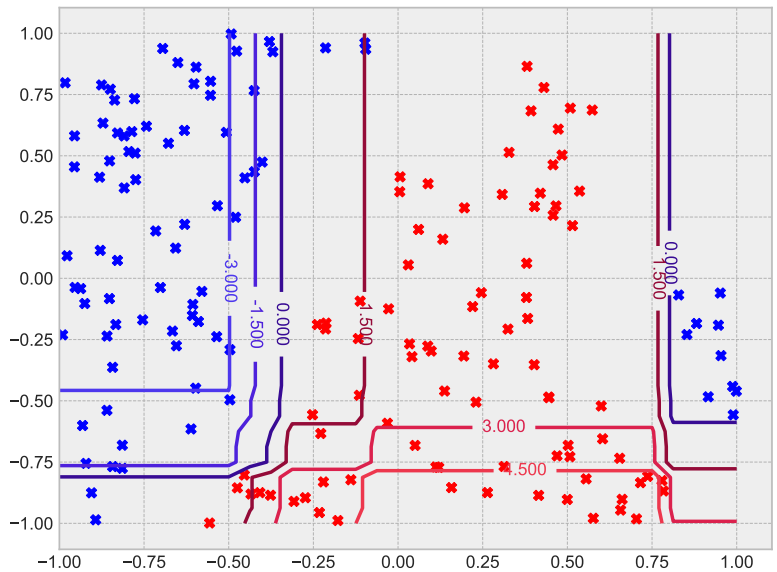
Example: boosted decision stumps.





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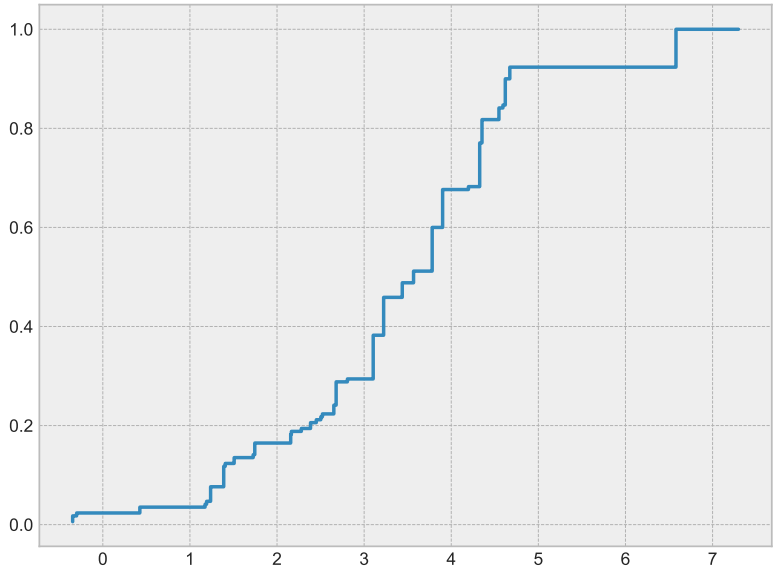

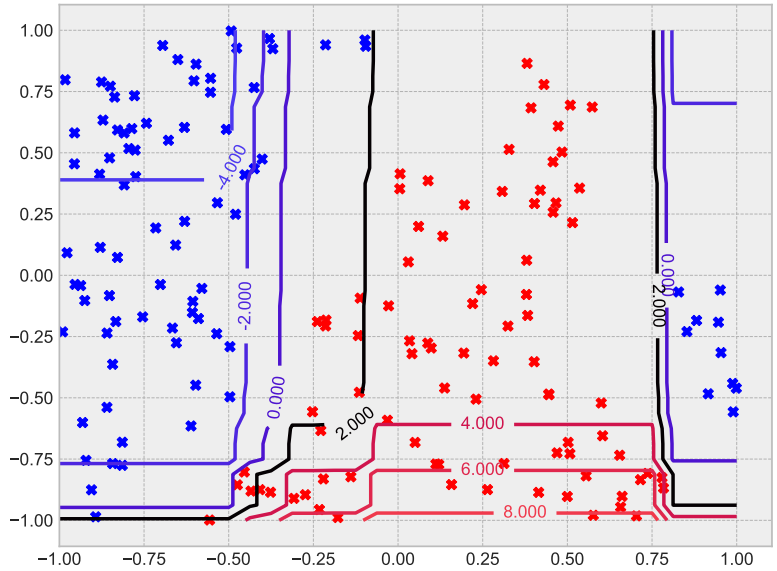

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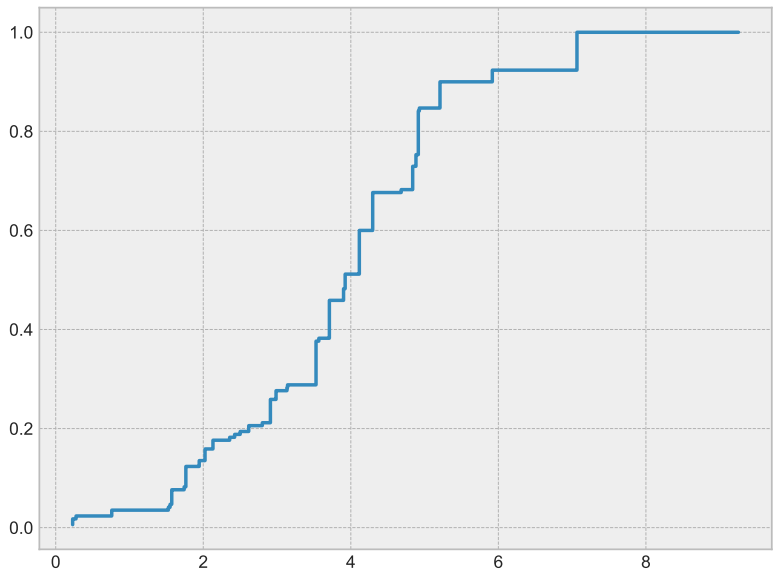

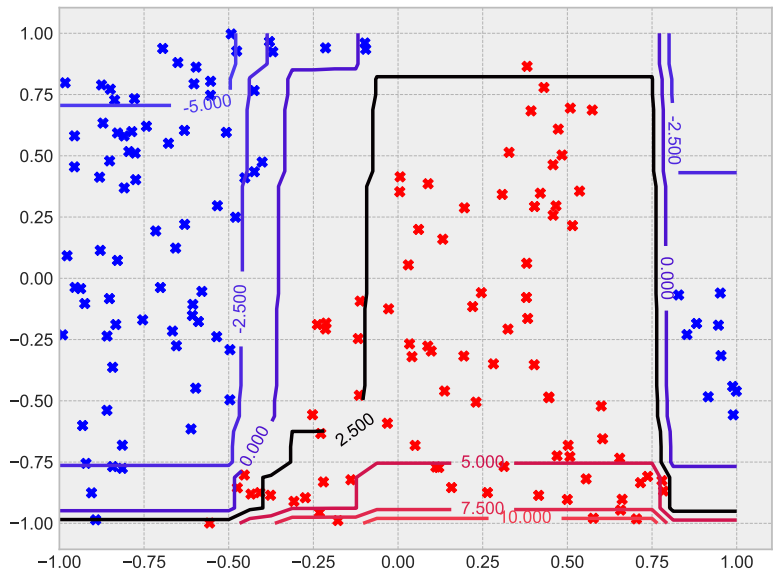

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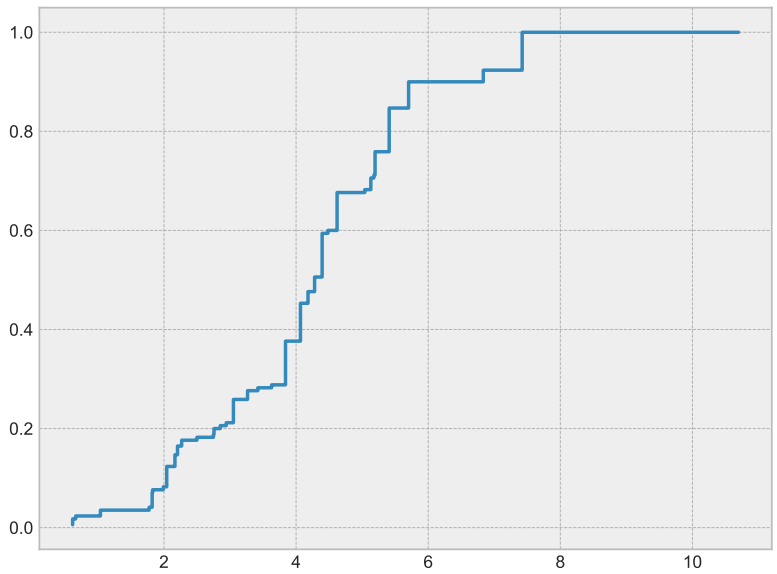

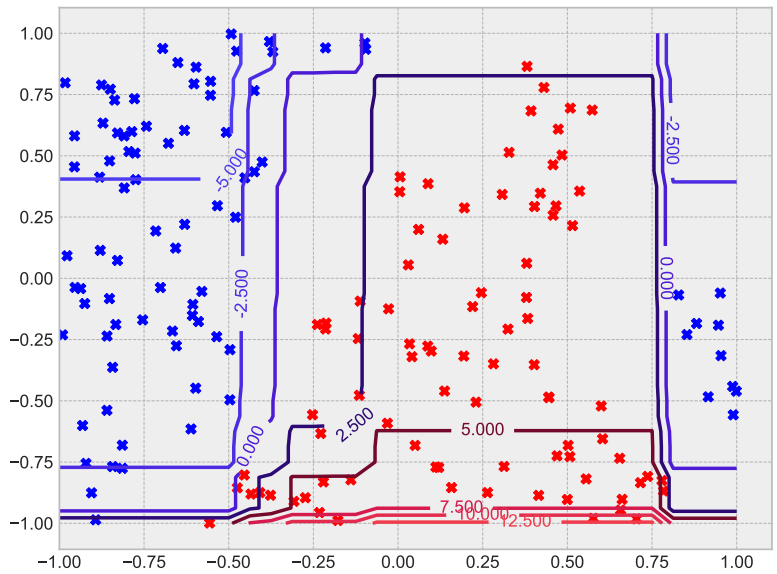

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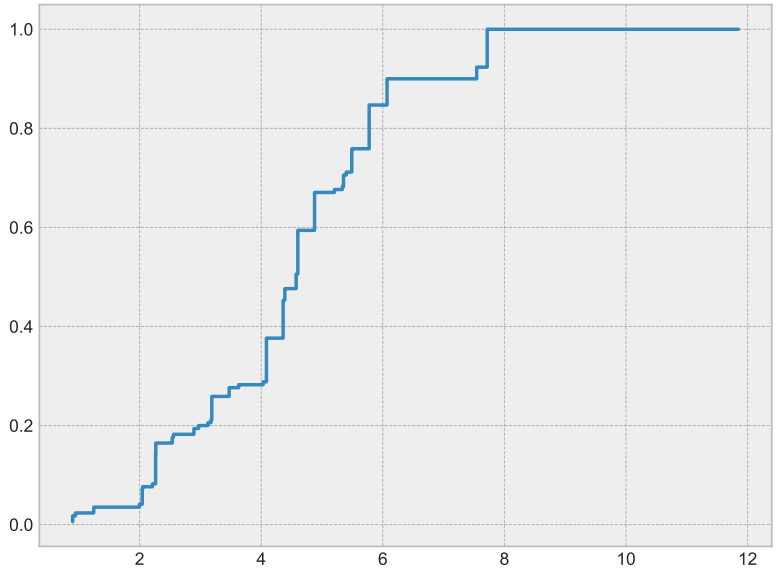
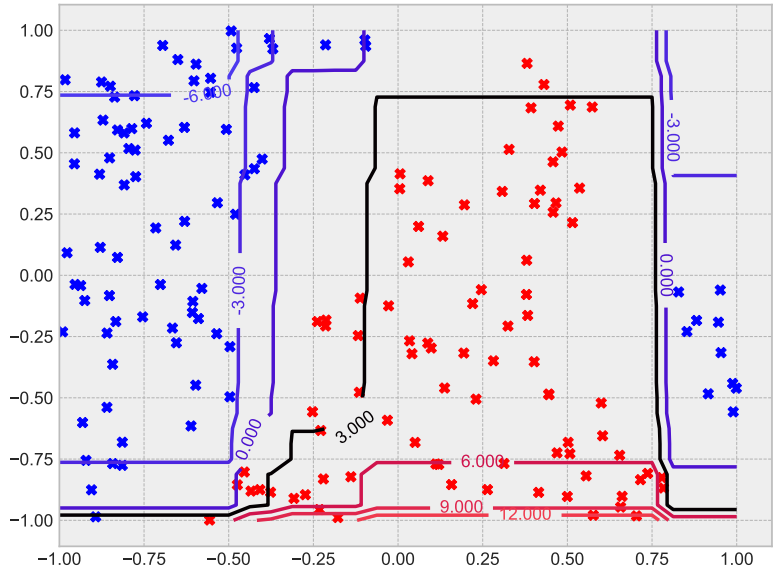
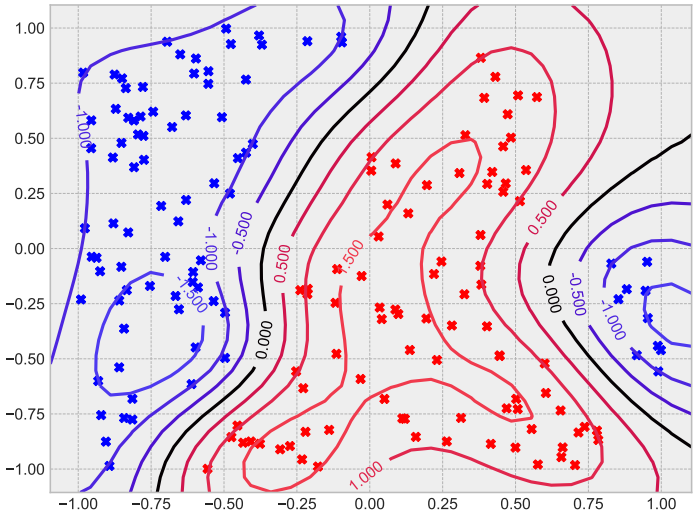
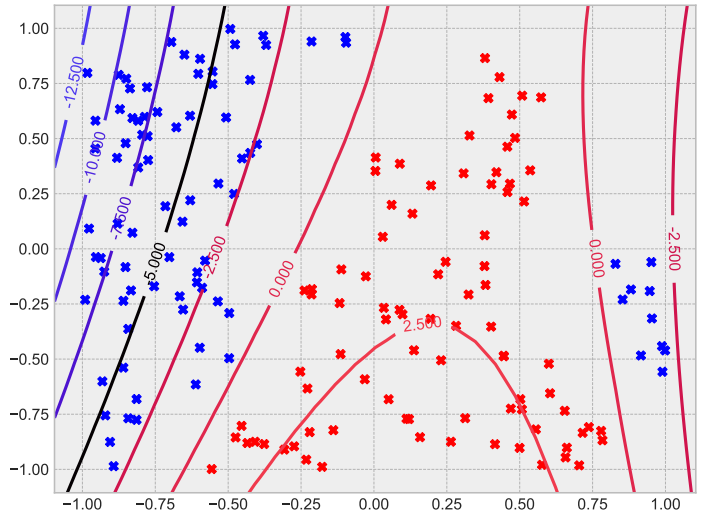




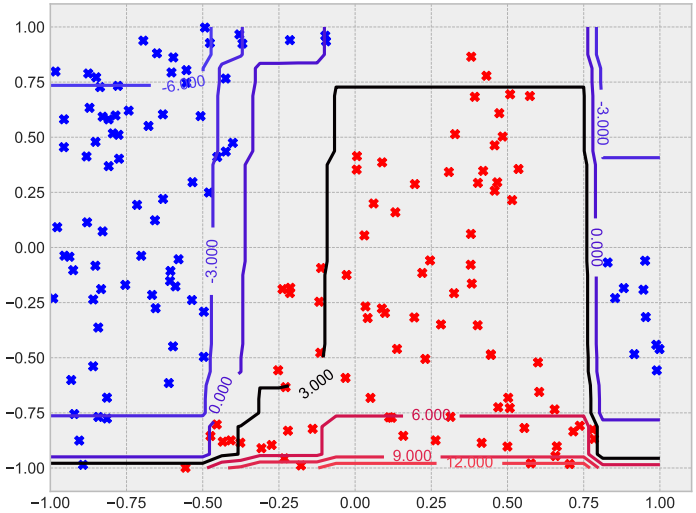
Margins appear throughout machine learning.



RBF SVM.



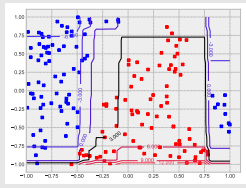
Quadratic SVM.



Boosted stumps.

?

ReLU network.



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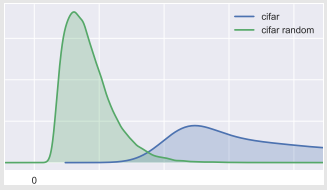
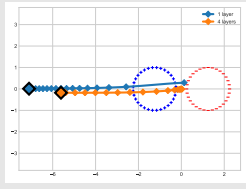
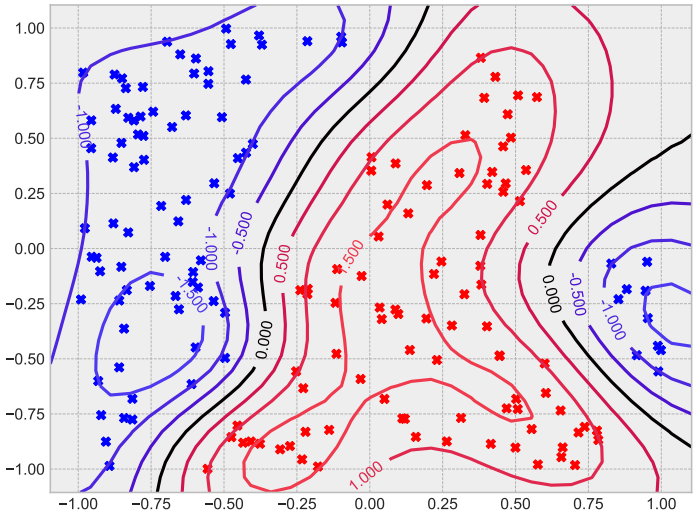


Generalization.



Optimization.

Margins appear throughout machine learning.



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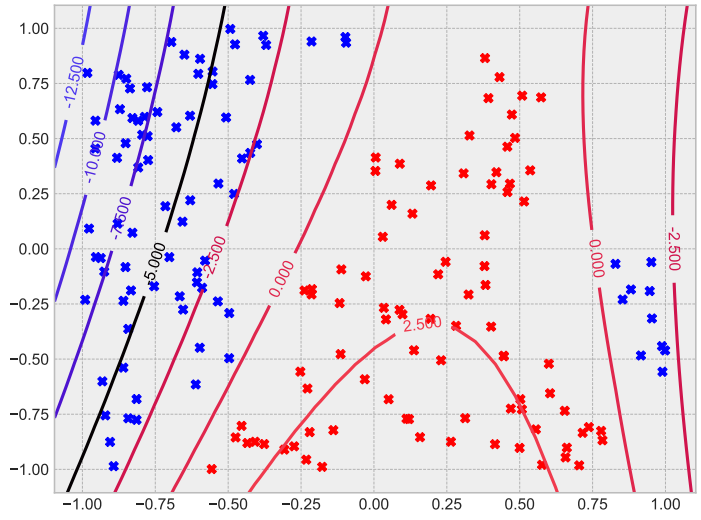
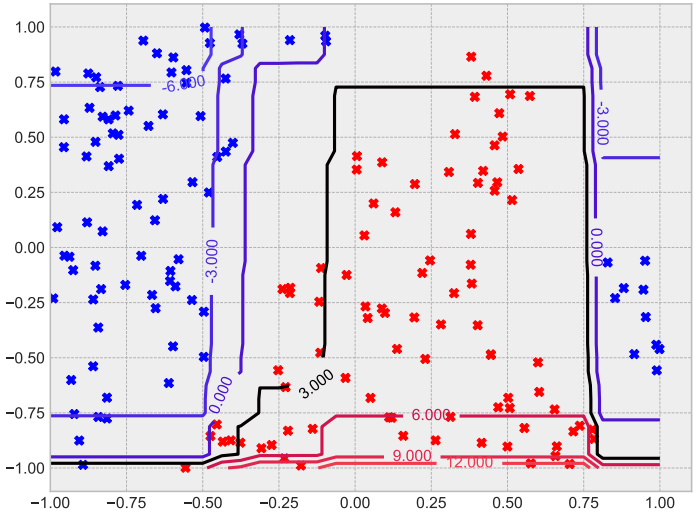


Quadratic SVM.



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ReLU network.

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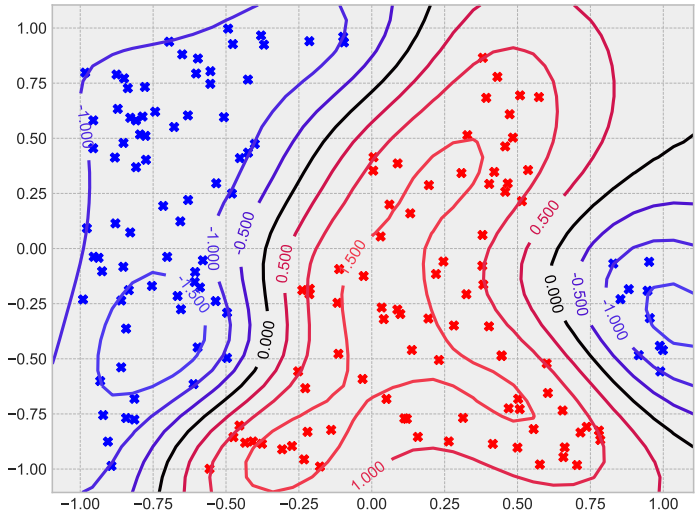

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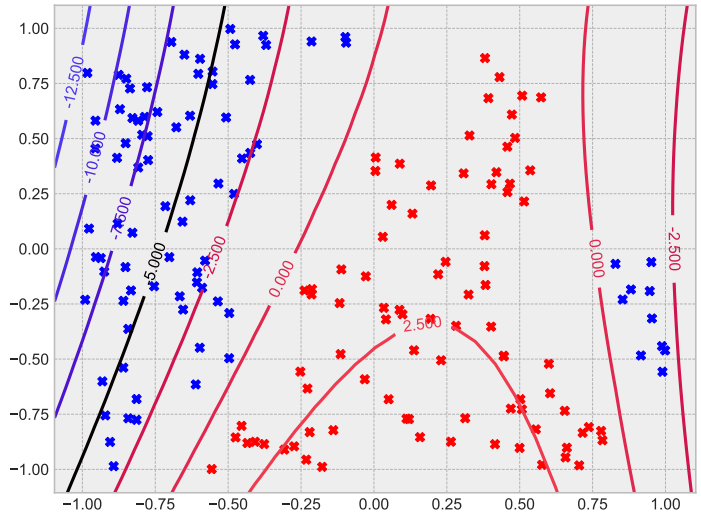

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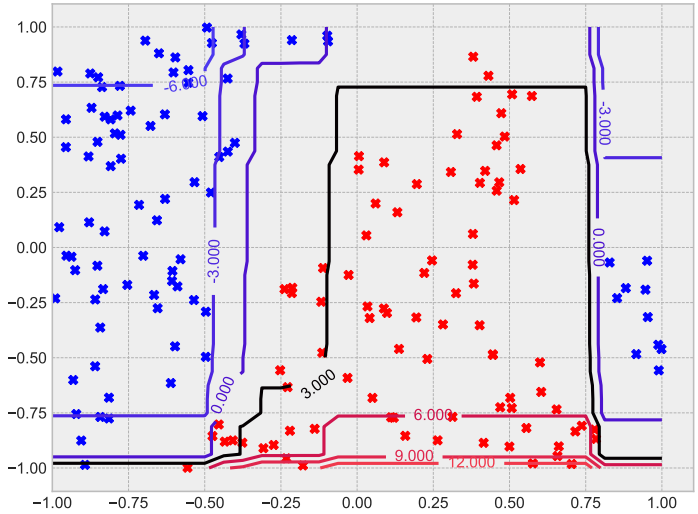

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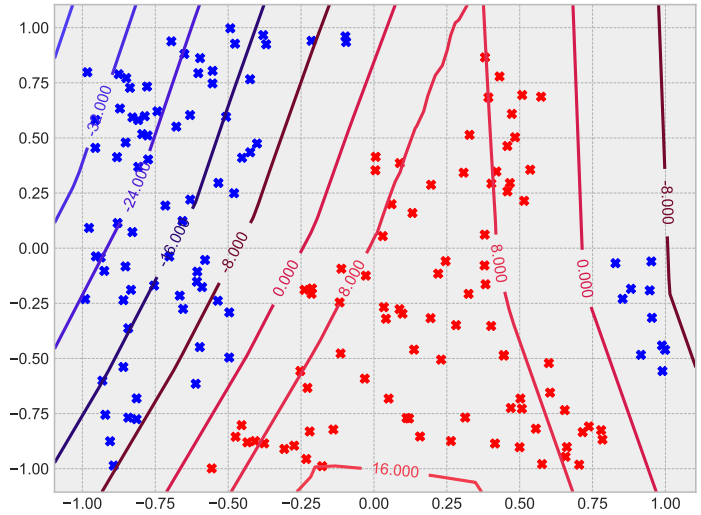

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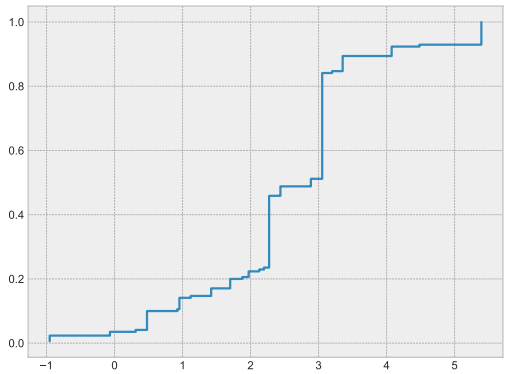

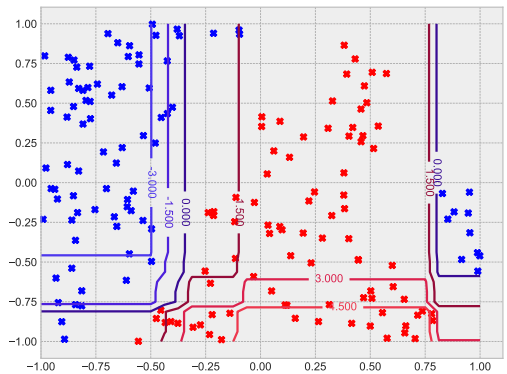

Boosted stumps.
($\mathcal{O}(n)$ param.)

Margin plots

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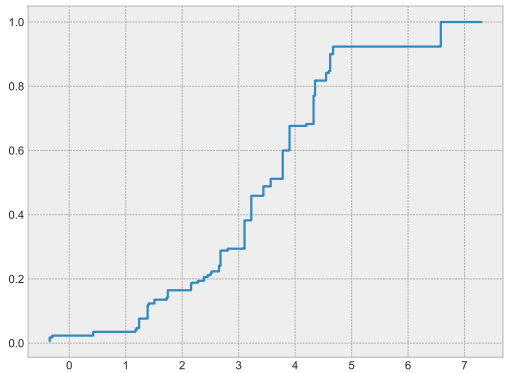

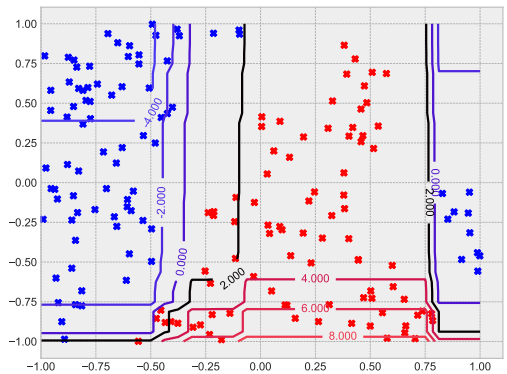

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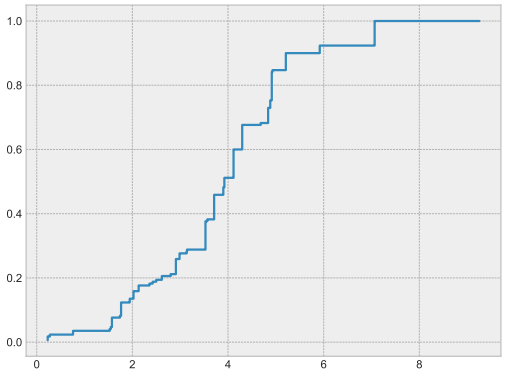

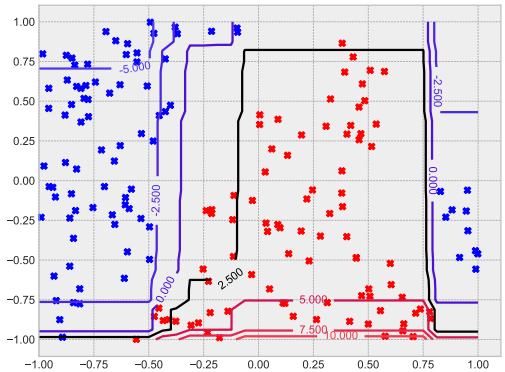

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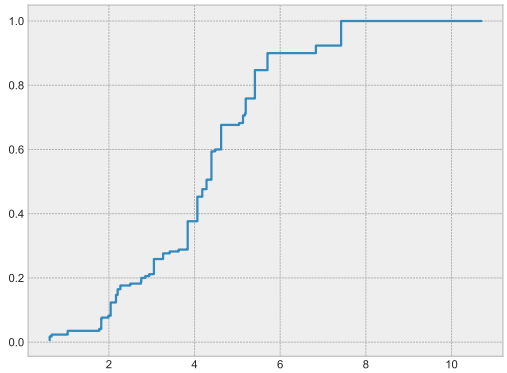

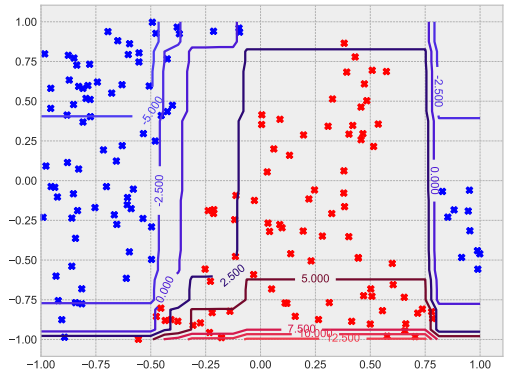

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($\mathcal{O}(n)$ param.)

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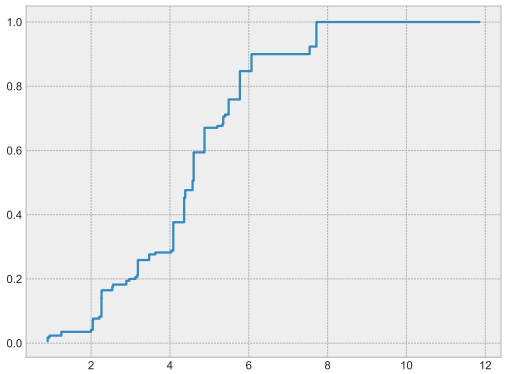

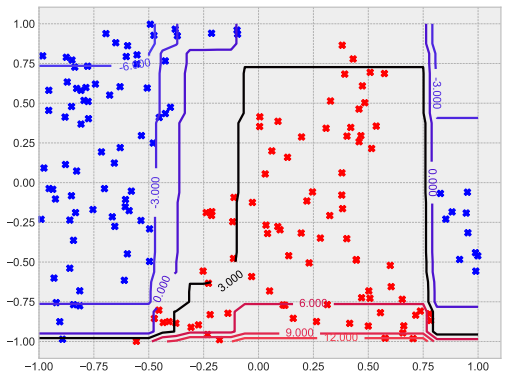

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Margin plots

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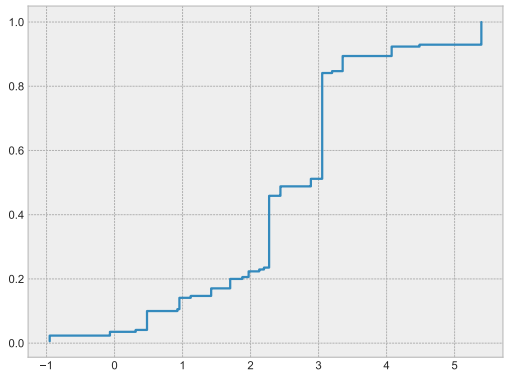

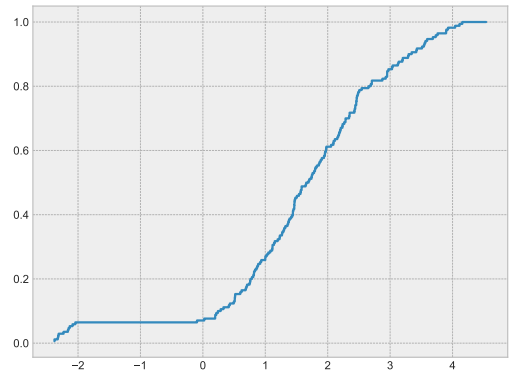

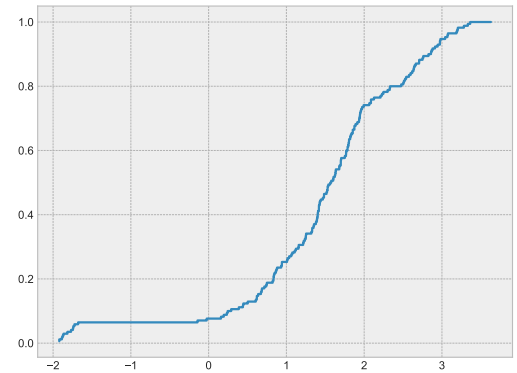

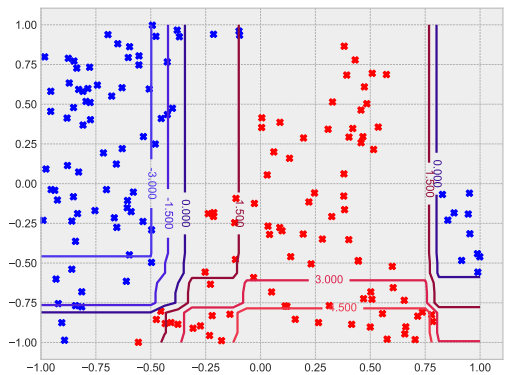

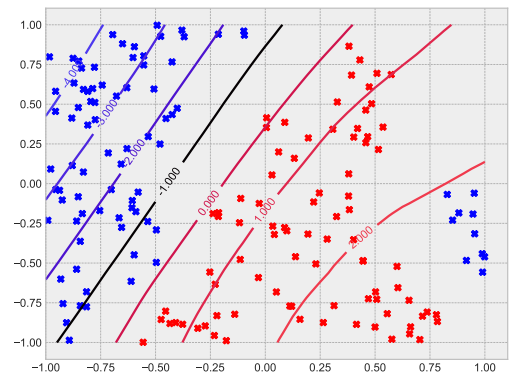

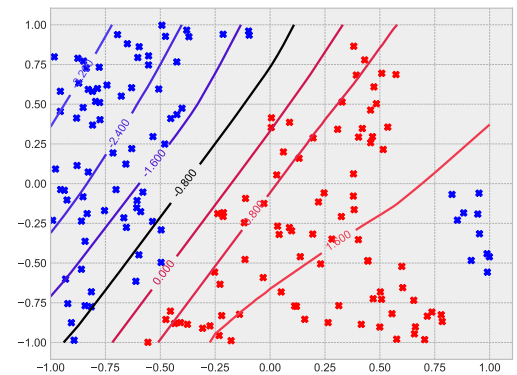

Boosted stumps.
($\mathcal{O}(n)$ param.)

2-layer ReLU.
($\mathcal{O}(n)$ param.)

3-layer ReLU.
($\mathcal{O}(n)$ param.)

Margin plots

Given $((x_i, y_i))_{i=1}^n$ and $f : \mathbb{R}^d \to \mathbb{R}^k$, plot distribution of

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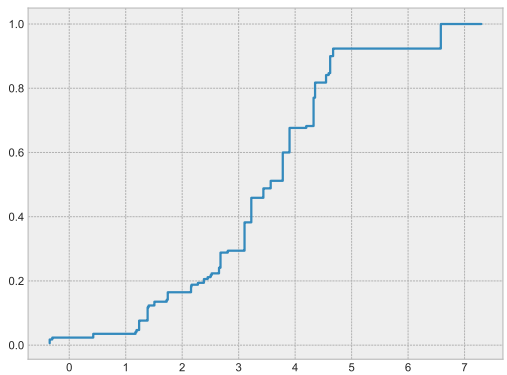
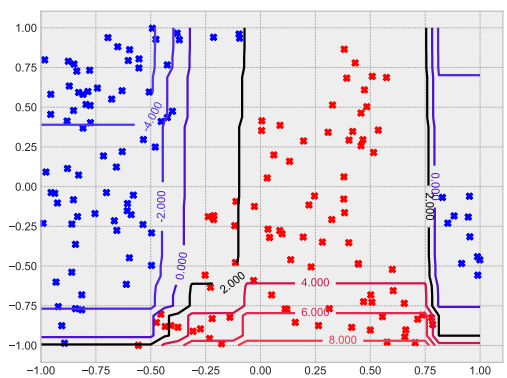
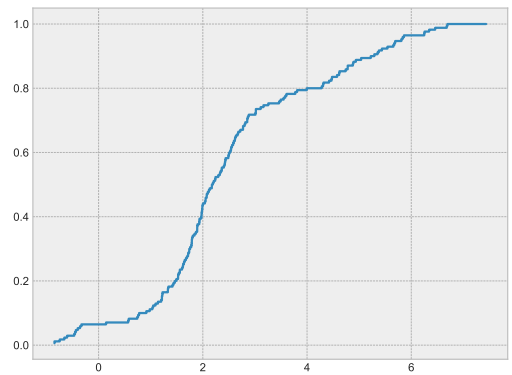
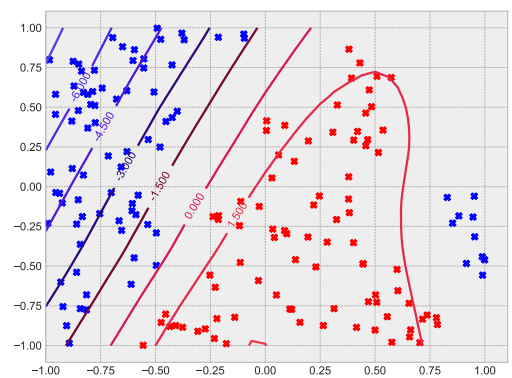


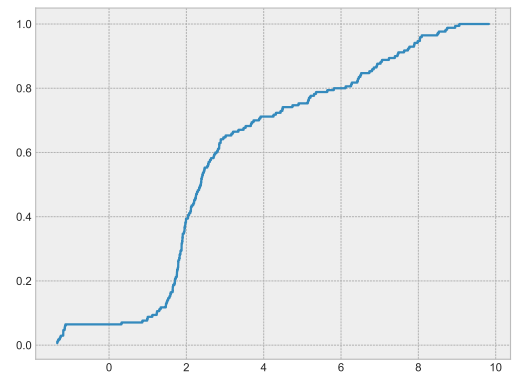


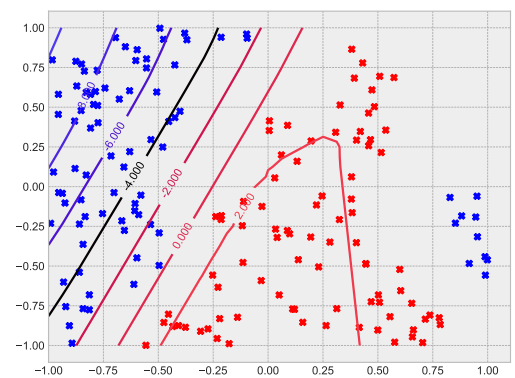
Boosted stumps.
($\mathcal{O}(n)$ param.)





2-layer ReLU.
($\mathcal{O}(n)$ param.)





3-layer ReLU.
($\mathcal{O}(n)$ param.)

Margin plots

Given $((x_i, y_i))_{i=1}^n$ and $f : \mathbb{R}^d \to \mathbb{R}^k$, plot distribution of

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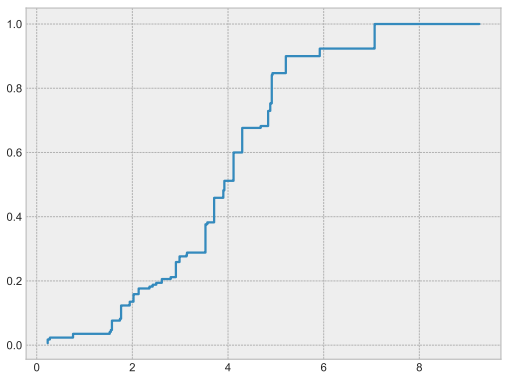
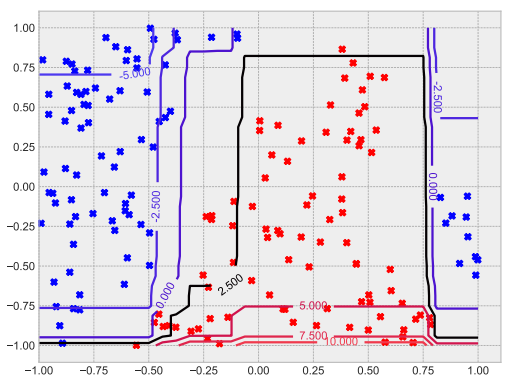
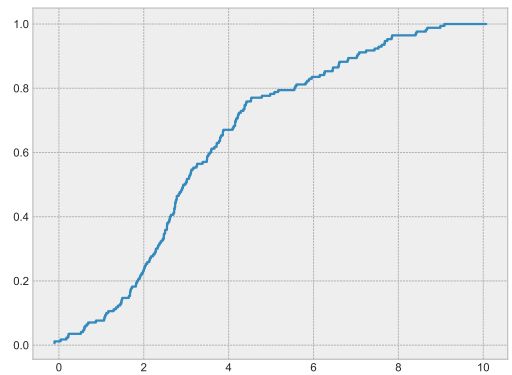
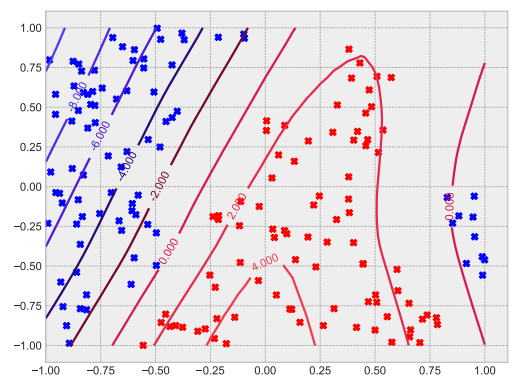


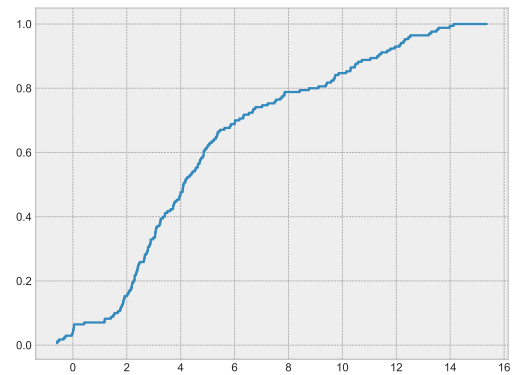


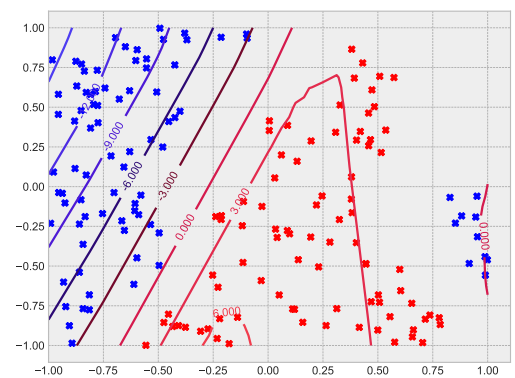
Boosted stumps.
($\mathcal{O}(n)$ param.)





2-layer ReLU.
($\mathcal{O}(n)$ param.)





3-layer ReLU.
($\mathcal{O}(n)$ param.)

Margin plots

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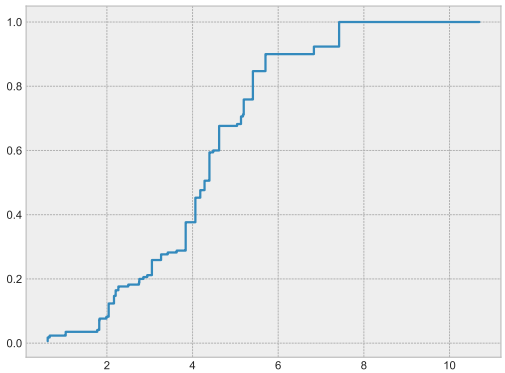

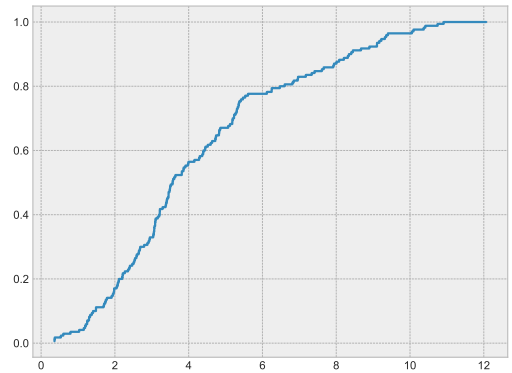

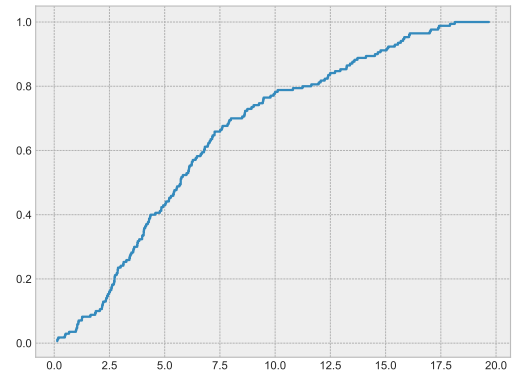

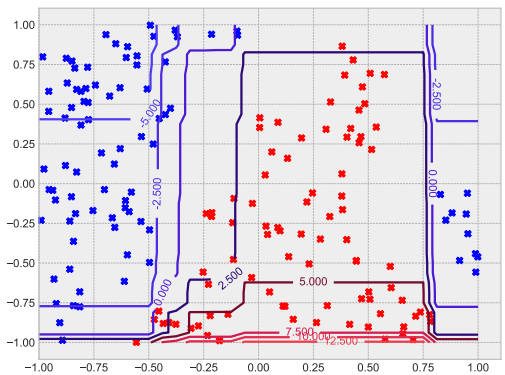

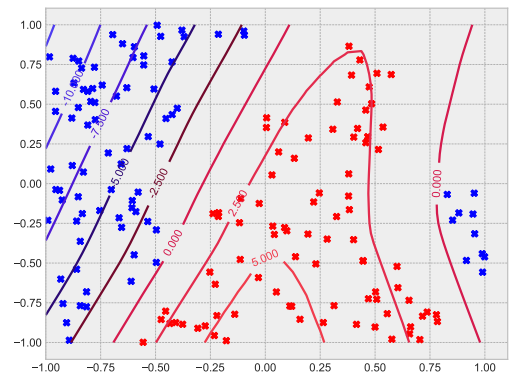

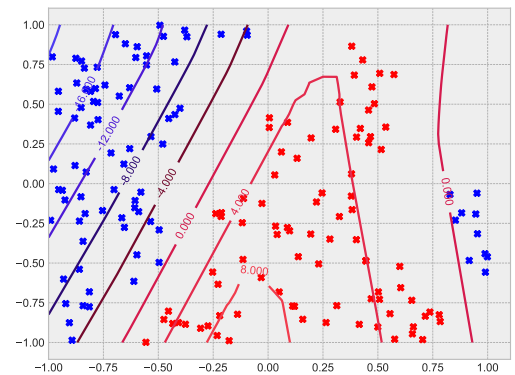

Boosted stumps.
($\mathcal{O}(n)$ param.)

2-layer ReLU.
($\mathcal{O}(n)$ param.)

3-layer ReLU.
($\mathcal{O}(n)$ param.)

Margin plots

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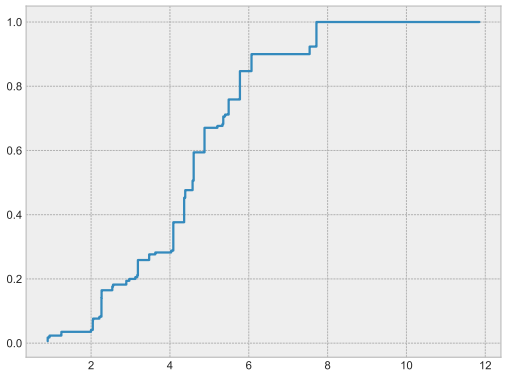
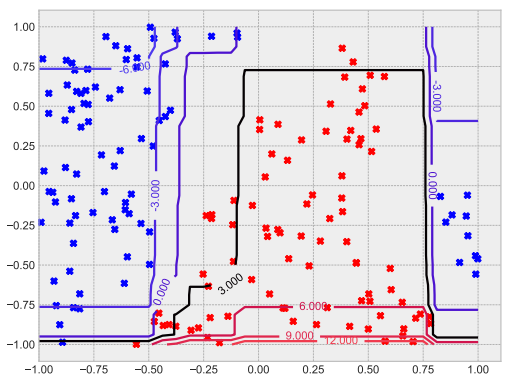
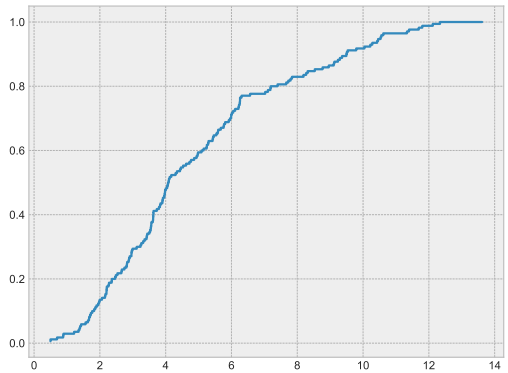
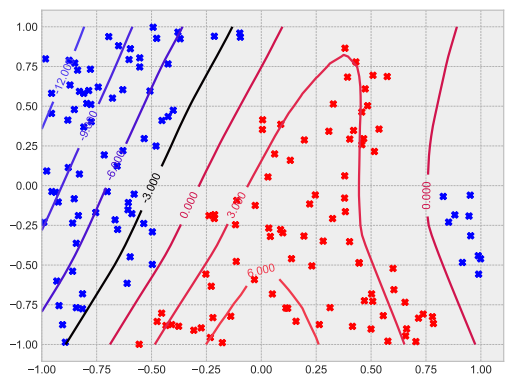


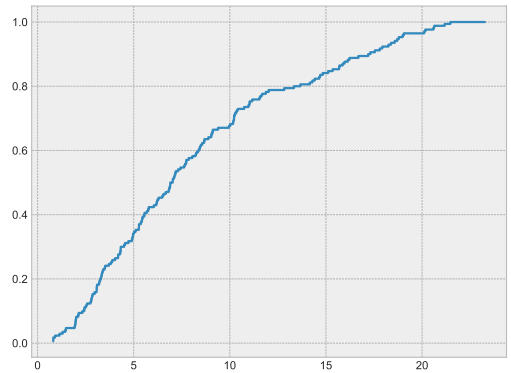


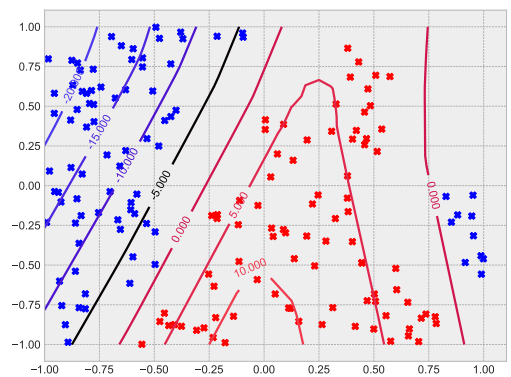
Boosted stumps.
($\mathcal{O}(n)$ param.)





2-layer ReLU.
($\mathcal{O}(n)$ param.)





3-layer ReLU.
($\mathcal{O}(n)$ param.)

Margin plots

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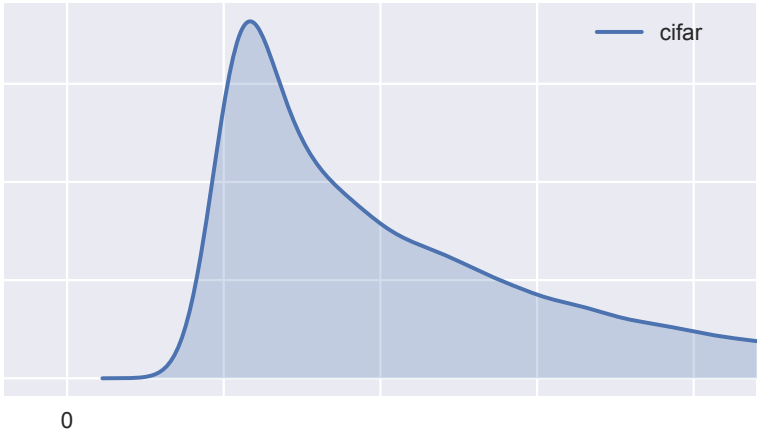

Unnormalized margins ($C_f = 1$).

Unnormalized margins can't distinguish random and true labels.

Margin plots

Given $((x_i, y_i))_{i=1}^n$ and $f : \mathbb{R}^d \to \mathbb{R}^k$, plot distribution of

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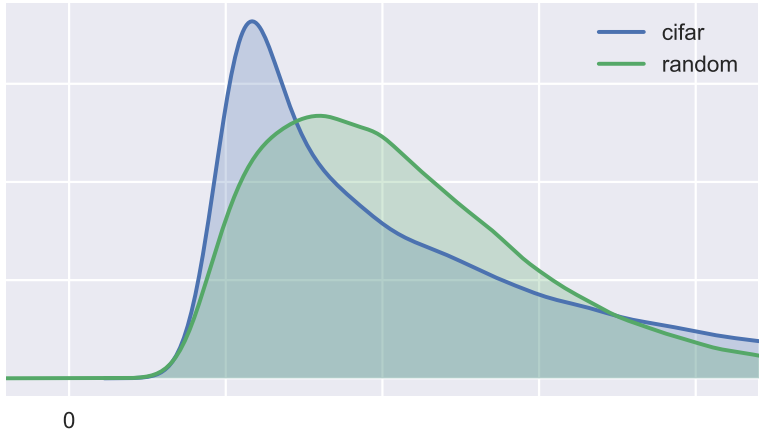

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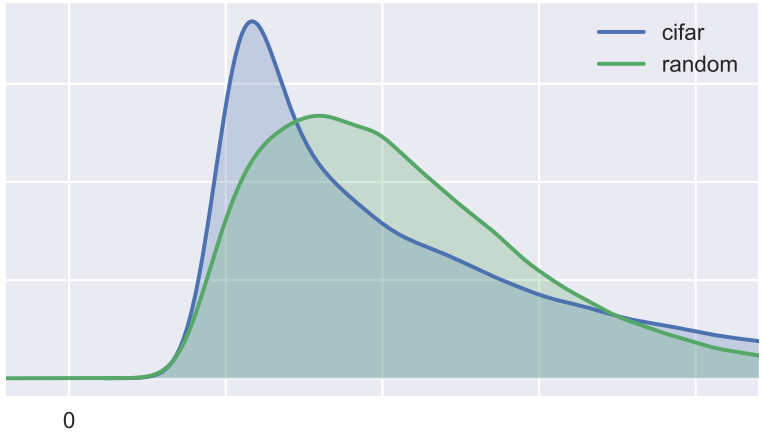

Unnormalized margins ($C_f = 1$).

Unnormalized margins can't distinguish random and true labels.

Margin plots

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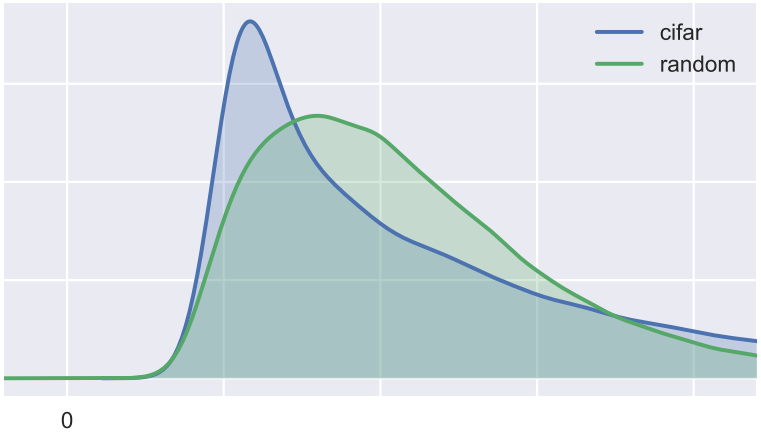

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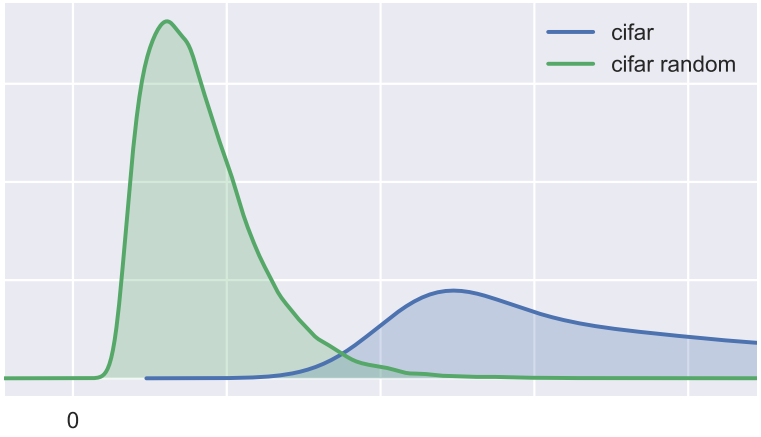

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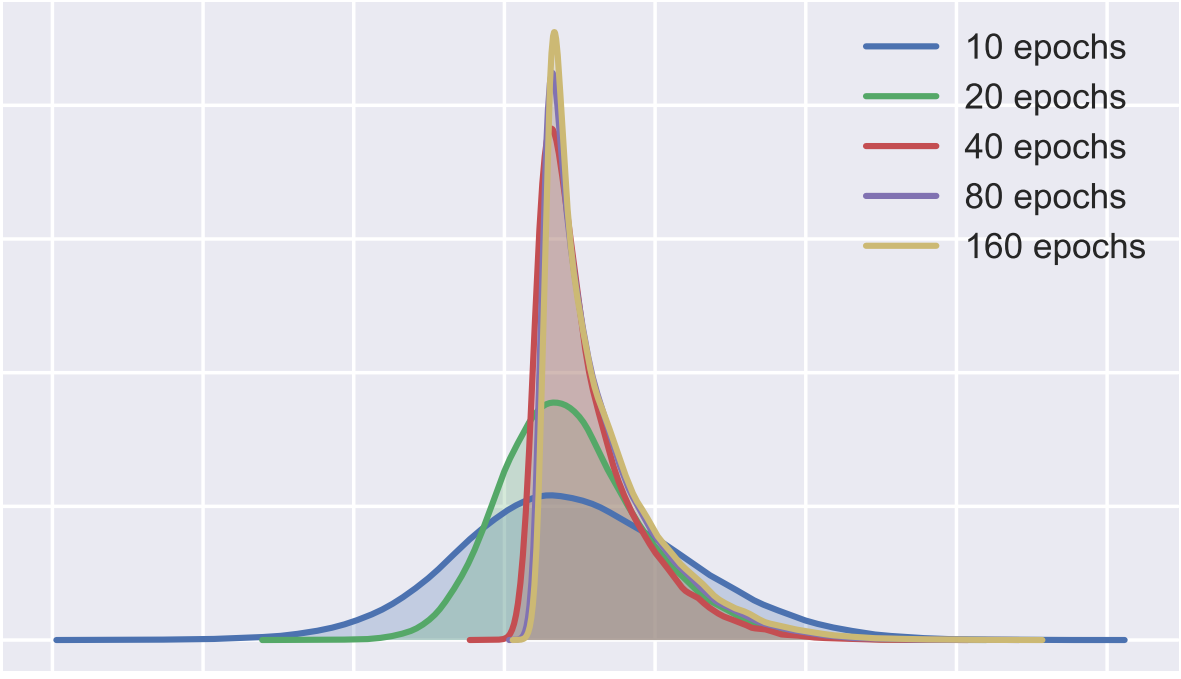

GD improves normalized margins!

Summary of margin plots. (Purely empirical.)

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What about a generalization bound?
(And how is it normalized?)

Theorem (Bartlett-Foster-Telgarsky, 2017).
Fix any architecture with ρ-Lipschitz σ_i, $\sigma_i(0) = 0$.
With probability $\geq 1 - \delta$ over data $X \in \mathbb{R}^{n \times d}$,
for any margin γ and weights $(W_i)_{i=1}^L$,

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Remarks.

- $\prod_i \rho_i \|W_i\|$ is (upper bound on) Lipschitz constant.
- *Predictive* of empirical performance. (Next slide.)
- No explicit combinatorial factors. (But $\|X\|_F \ldots$)
- Multivariate gates (e.g., ReLU+maxpool) and output.

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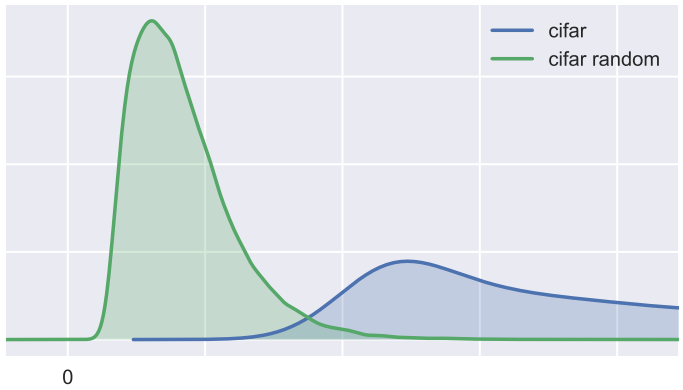

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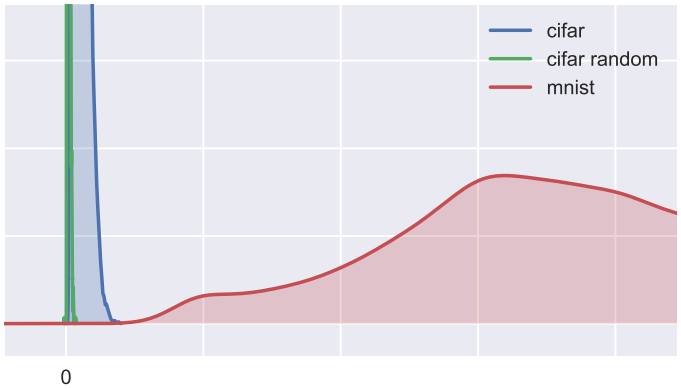

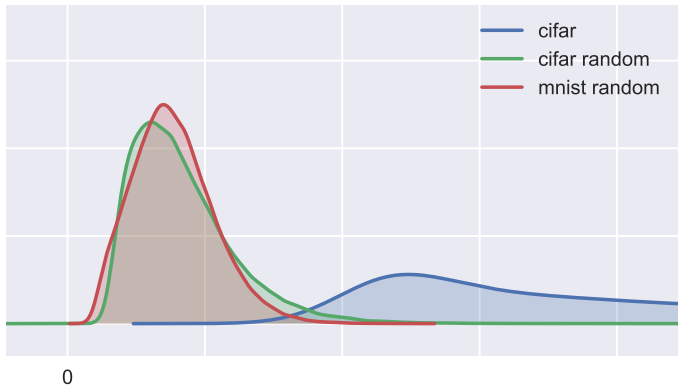

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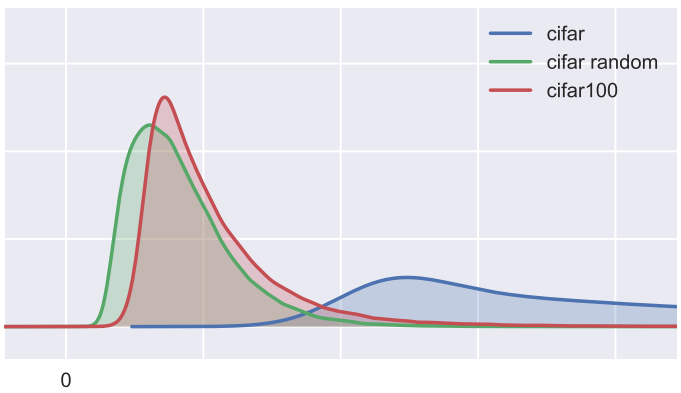

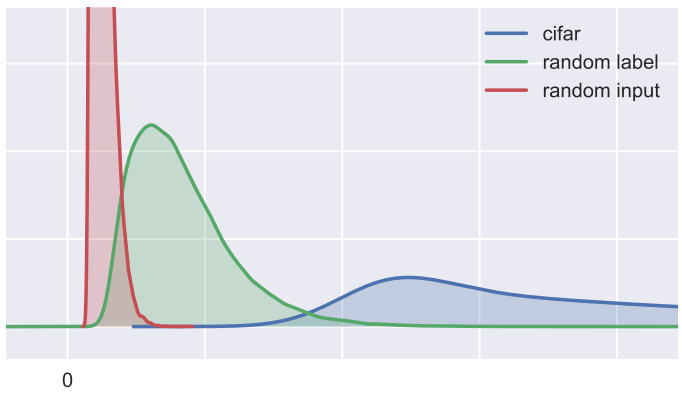

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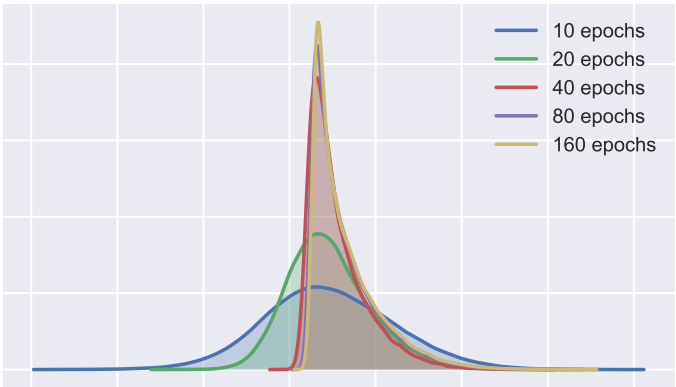

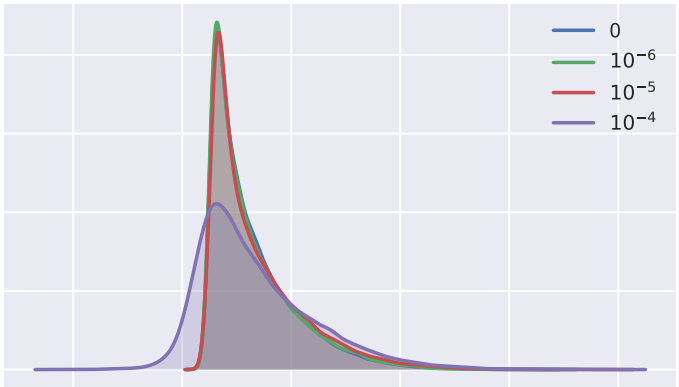

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Negative remark: "nuisance term".

- Not in (linear!) lower bound.
- Linear lower bound has aligned matrices,
  upper bound has "maximally misaligned" matrices;
  "misaligned nonlinearities" quickly increase #pieces.
- Ratio term $\lesssim L^{3/2} w \approx L\sqrt{p}$; useless for ResNet, RNNs, etc.

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Proof:
Layer-by-layer "matrix covering"
(avoids combinatorial parameters).

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"Uniform devations?"

- This methodology equally controls all predictors in some set.
- Set can be made small
  via sensitivity to data, predictors, and algorithm.

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Follow-up work and open problems.

- How to avoid degradation with depth and width?
- (Wei-Ma '19) and (Nagarajan-Kolter '19)
  depend on Jacobian matrices
  and bounds on within-network representations.
- (Golowich-Rakhlin-Shamir '18) improve dependency on Lipschitz, but $\sqrt{n}$ becomes $n^{1/5}$.

Comparison: VC Theory.

Theorem (Bartlett-Harvey-Liaw-Mehrabian '17).
Fix a ReLU architecture with L layers, p params.

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- This is "tight"; but $p > n$ in standard setups.
- Even though loose,
  proofs still illuminative.
- With threshold gates, becomes $\widetilde{\mathcal{O}}(p)$.
  Polynomial gates: $\widetilde{\mathcal{O}}(pL^2)$.
  Sigmoid: $\widetilde{\mathcal{O}}(m^2p^2)$ where m is # nodes.
  Arbitrary convex-concave: ∞.

Generalization summary.

- Empirically, GD seems to find large margin networks.
- Existing margin generalization bounds seem to correlate with observed generalization, but are still very loose.
- All existing bounds too sensitive to p and L...

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- Further understanding of gradient descent needed to better pin down "practically observed" networks.
- Going beyond classification?
- Regularization?

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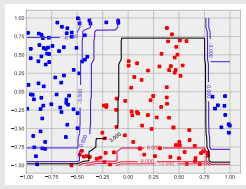
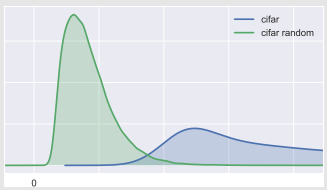
This lecture:

still need to *prove* gradient descent finds large margin networks.



Margins.



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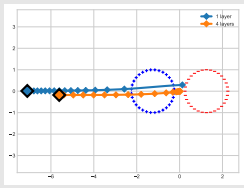

Optimization.

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- What about something deeper?

Deep linear networks

No nonlinearities:

$$x \mapsto W_L \cdots W_1 x.$$

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- Linear in the input x;
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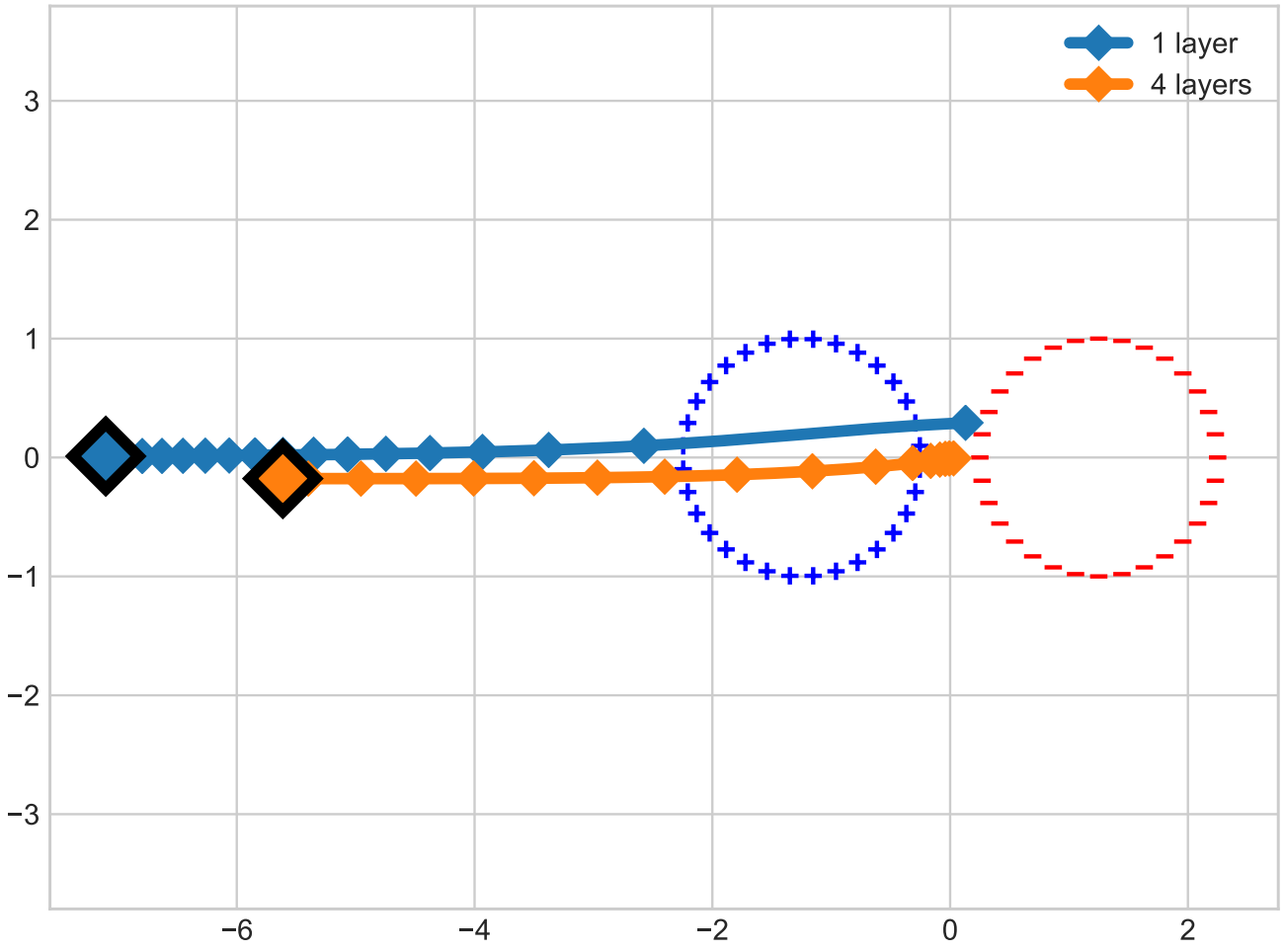
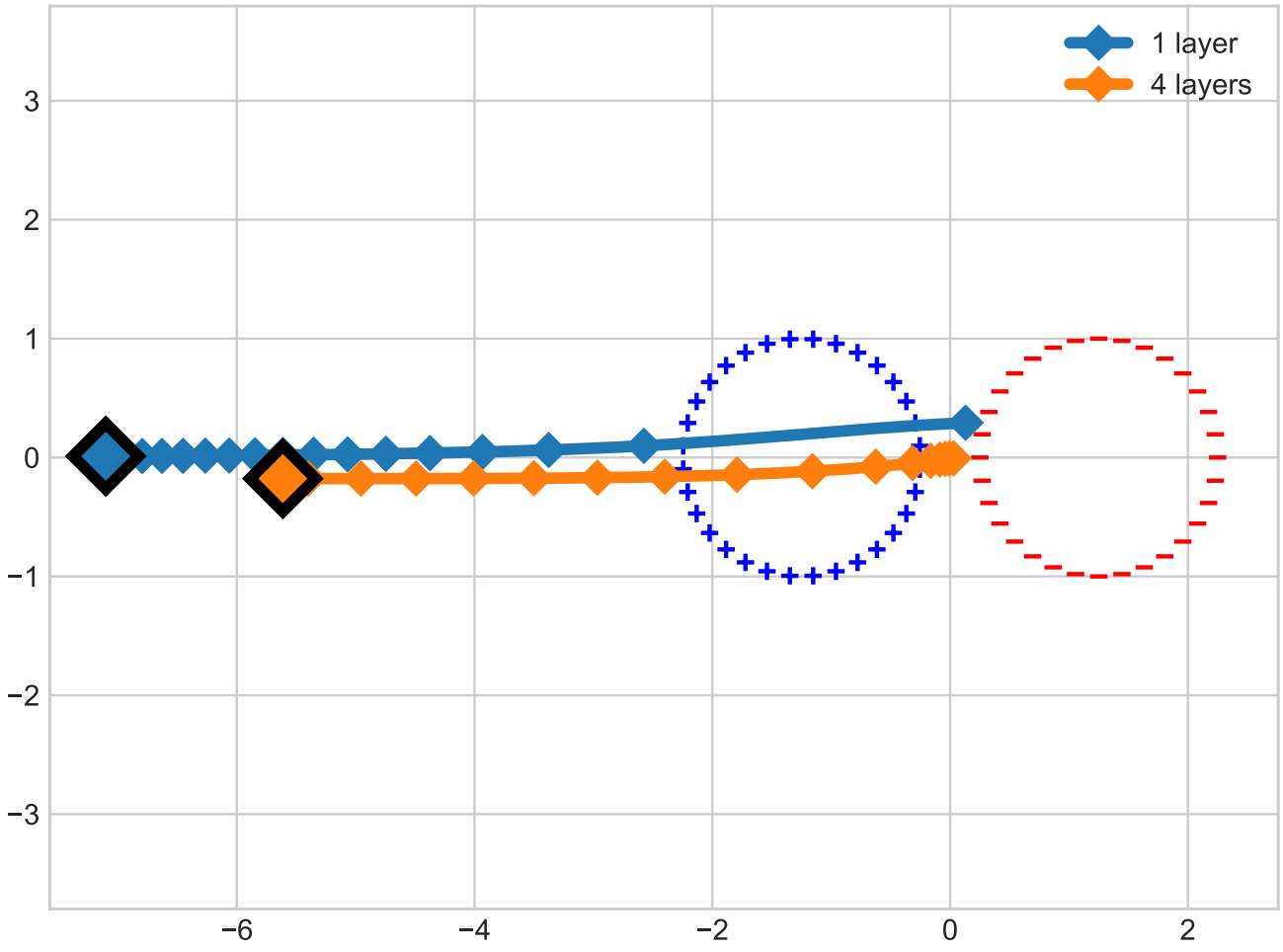
- Linear in the input x;
  multi-linear/polynomial in parameters $(W_L, \ldots, W_1)$.
- Not convex! What can we hope for?

Margin maximization..



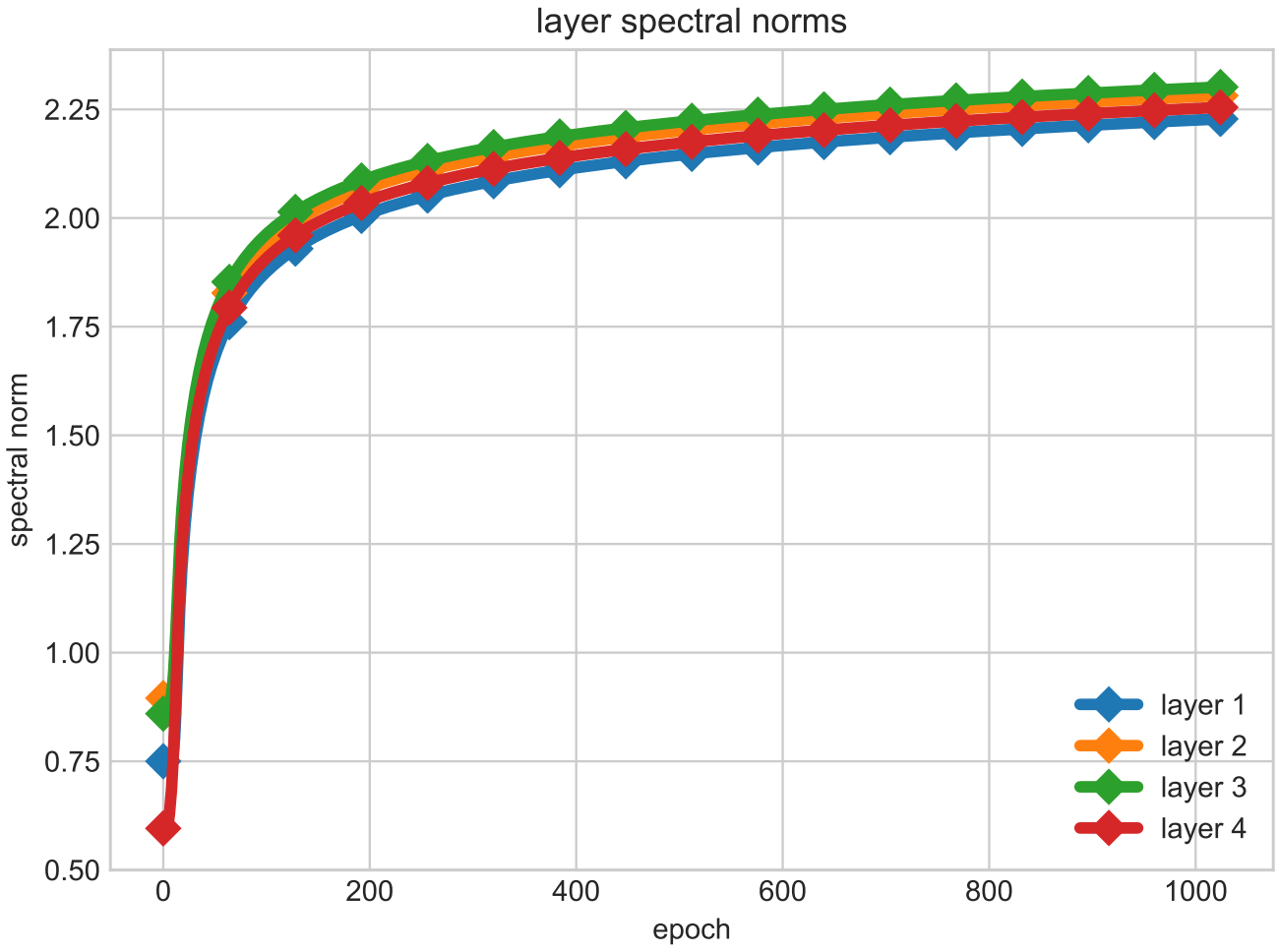
Margin maximization..



(This implies *at least one* weight matrix $\uparrow \infty$.)

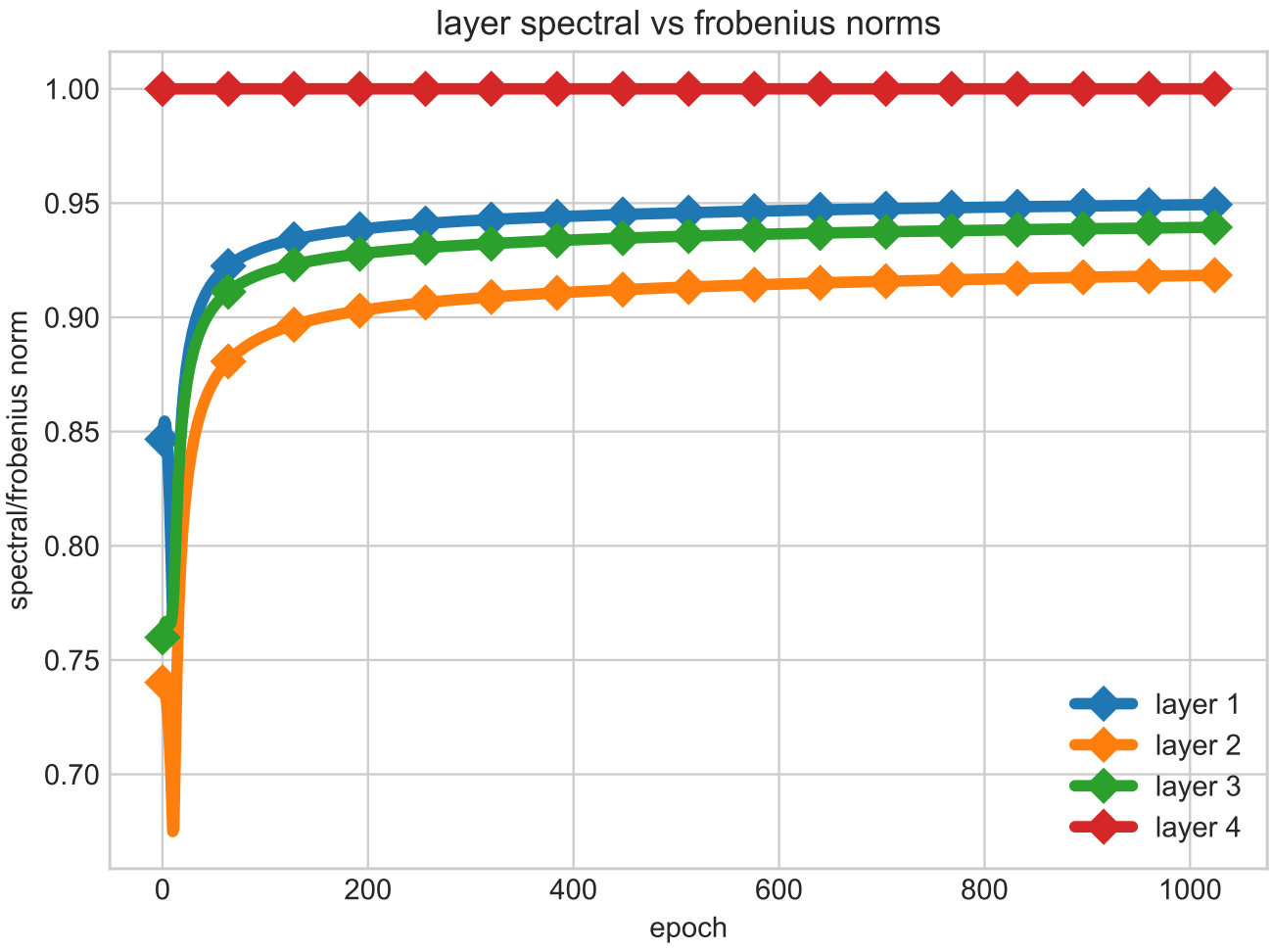
What do individual weight matrices do?

$\|W_i\|_2 \to \infty$ **for all layers** i**...** (simultaneously!)...



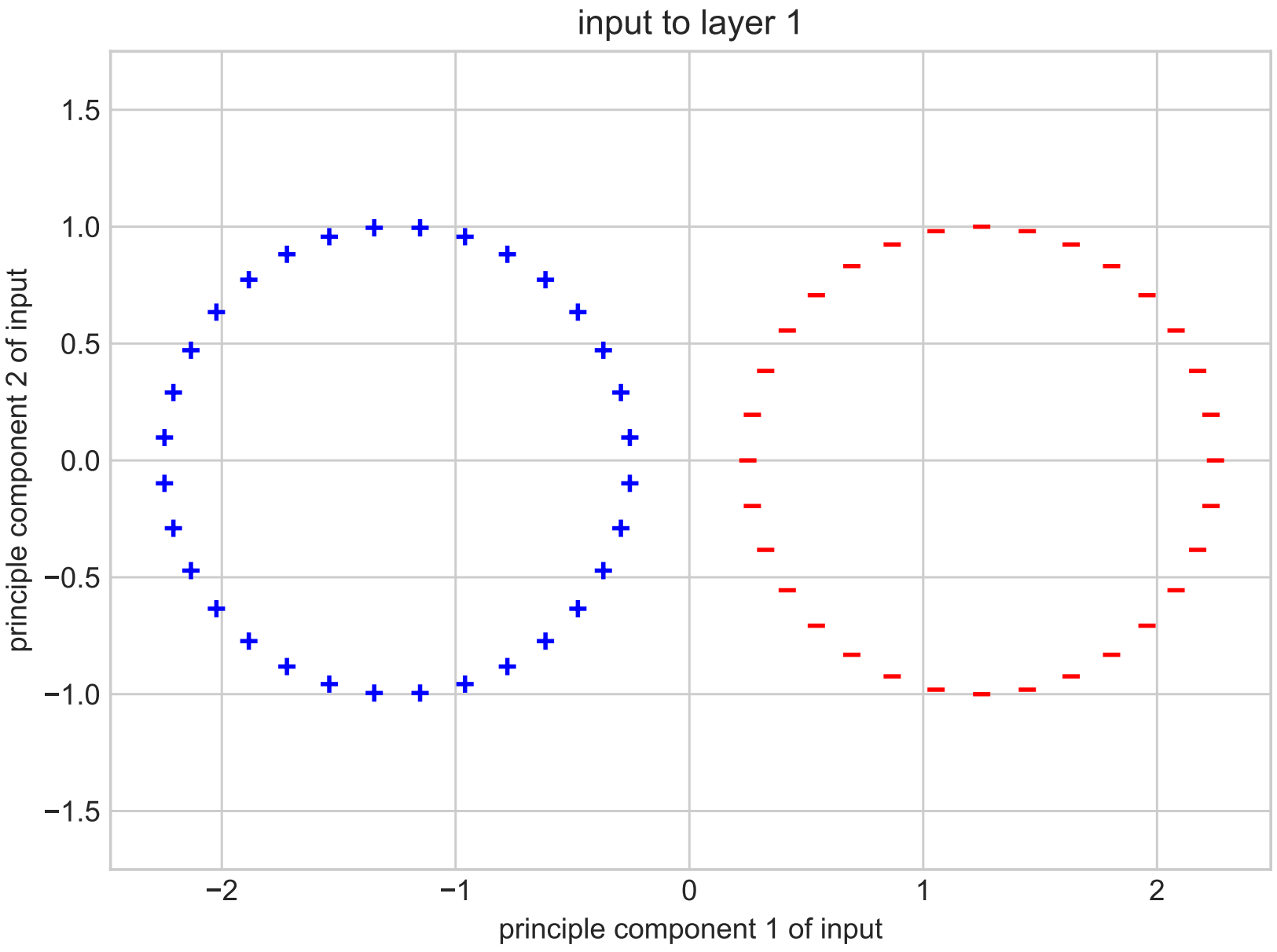
What are their ranks?

Layers are asymptotically rank 1!



Are they "wasting norm" layer-to-layer?

The layers *are aligned*.



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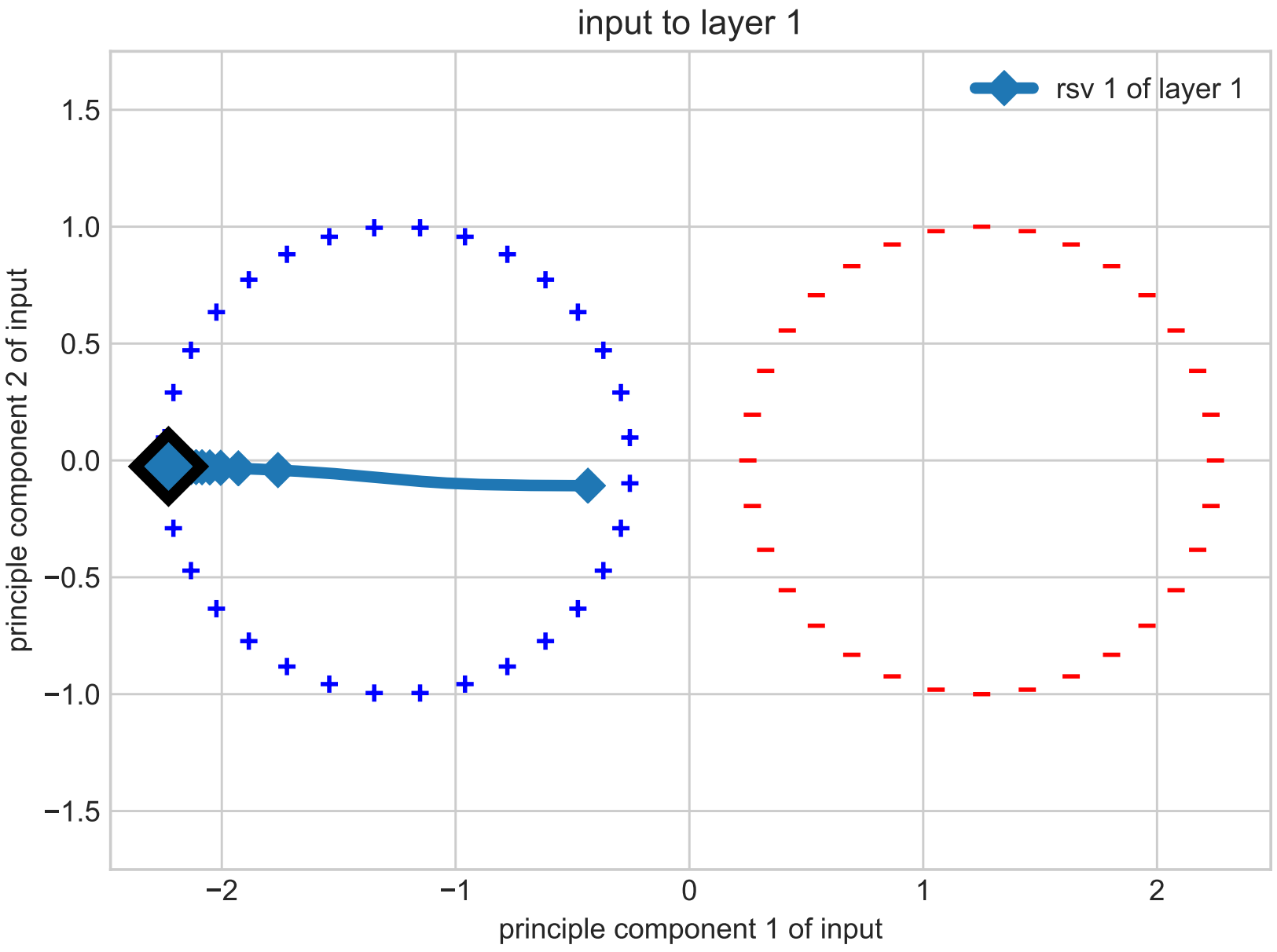

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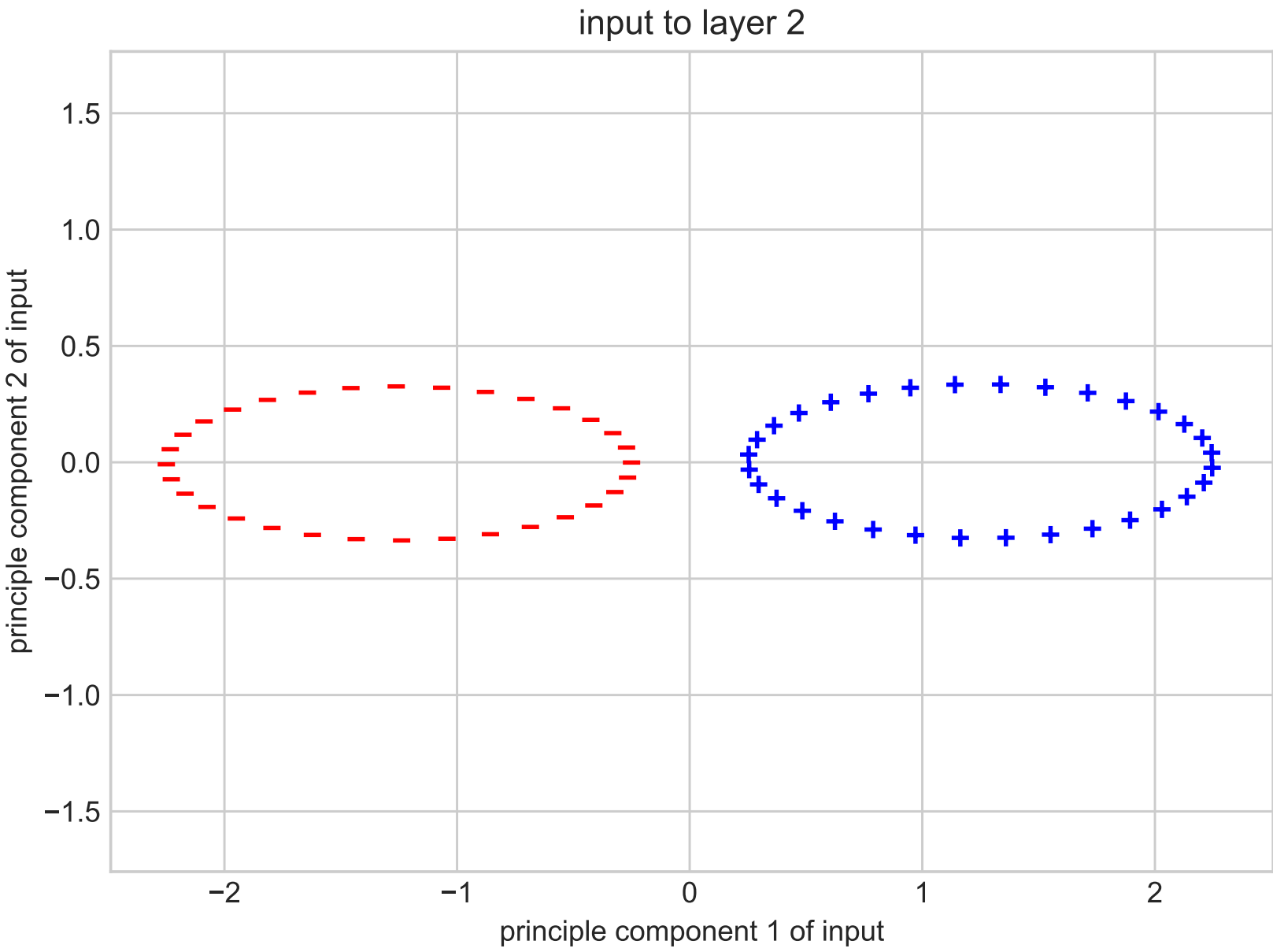

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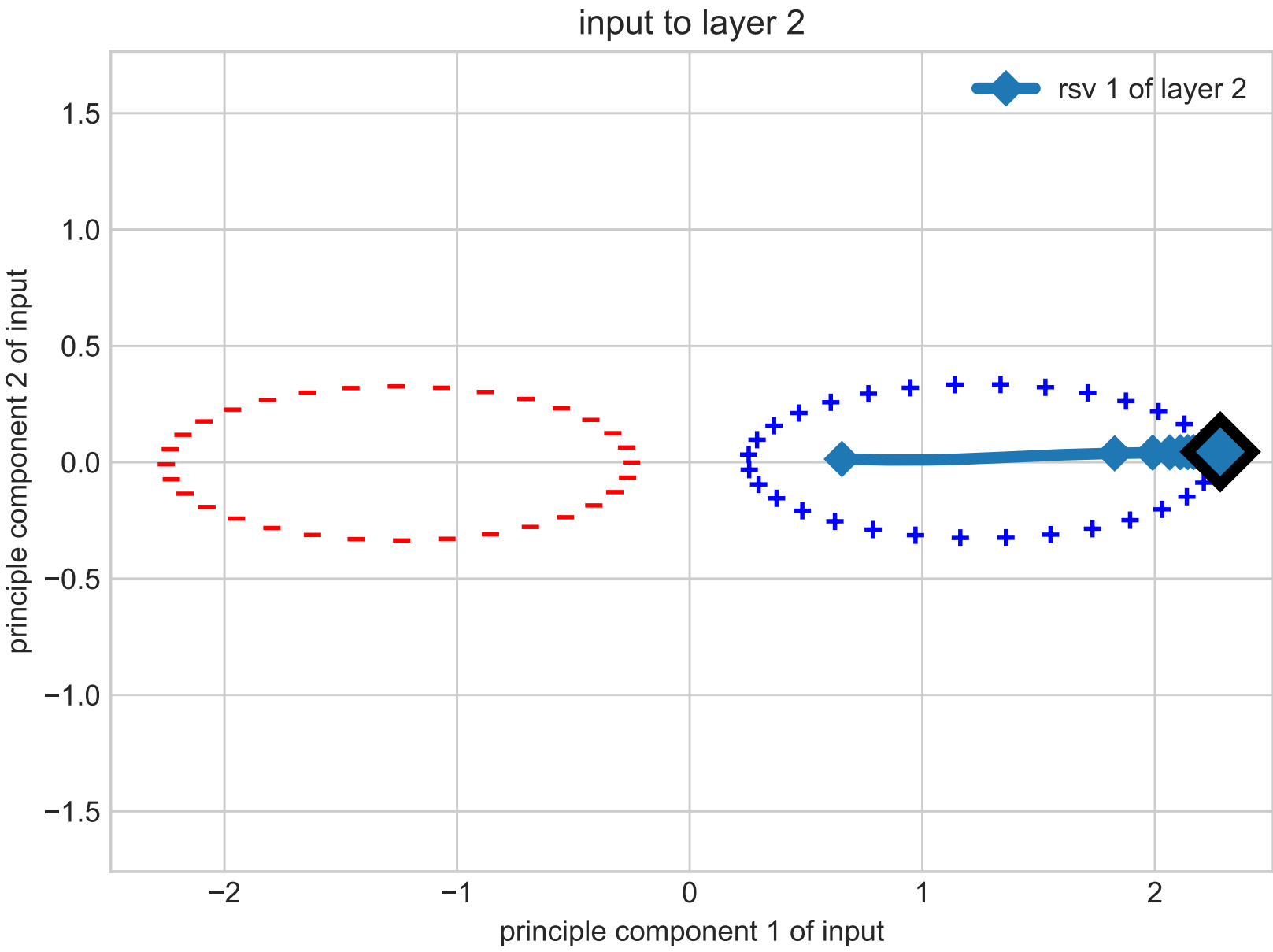

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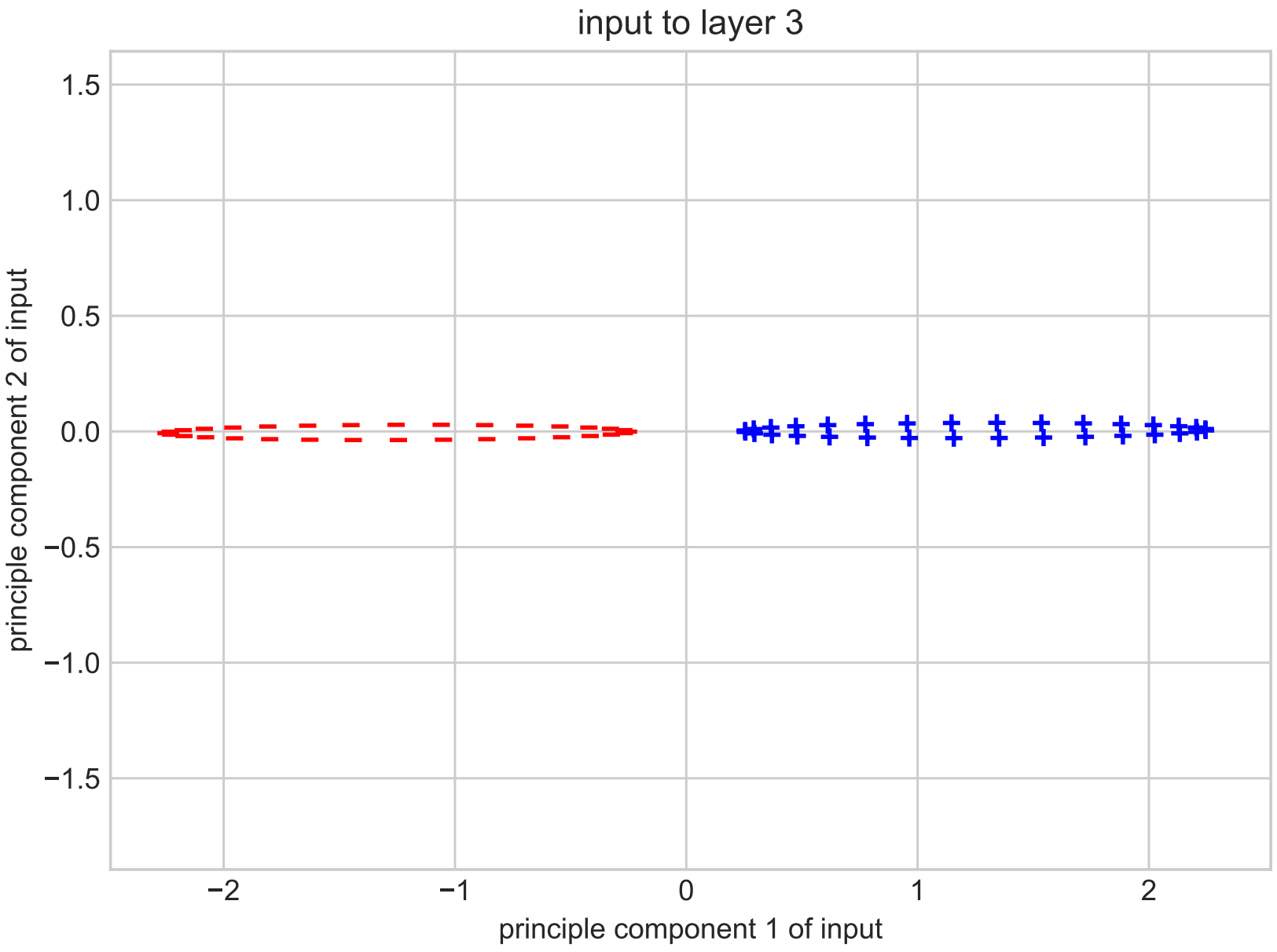

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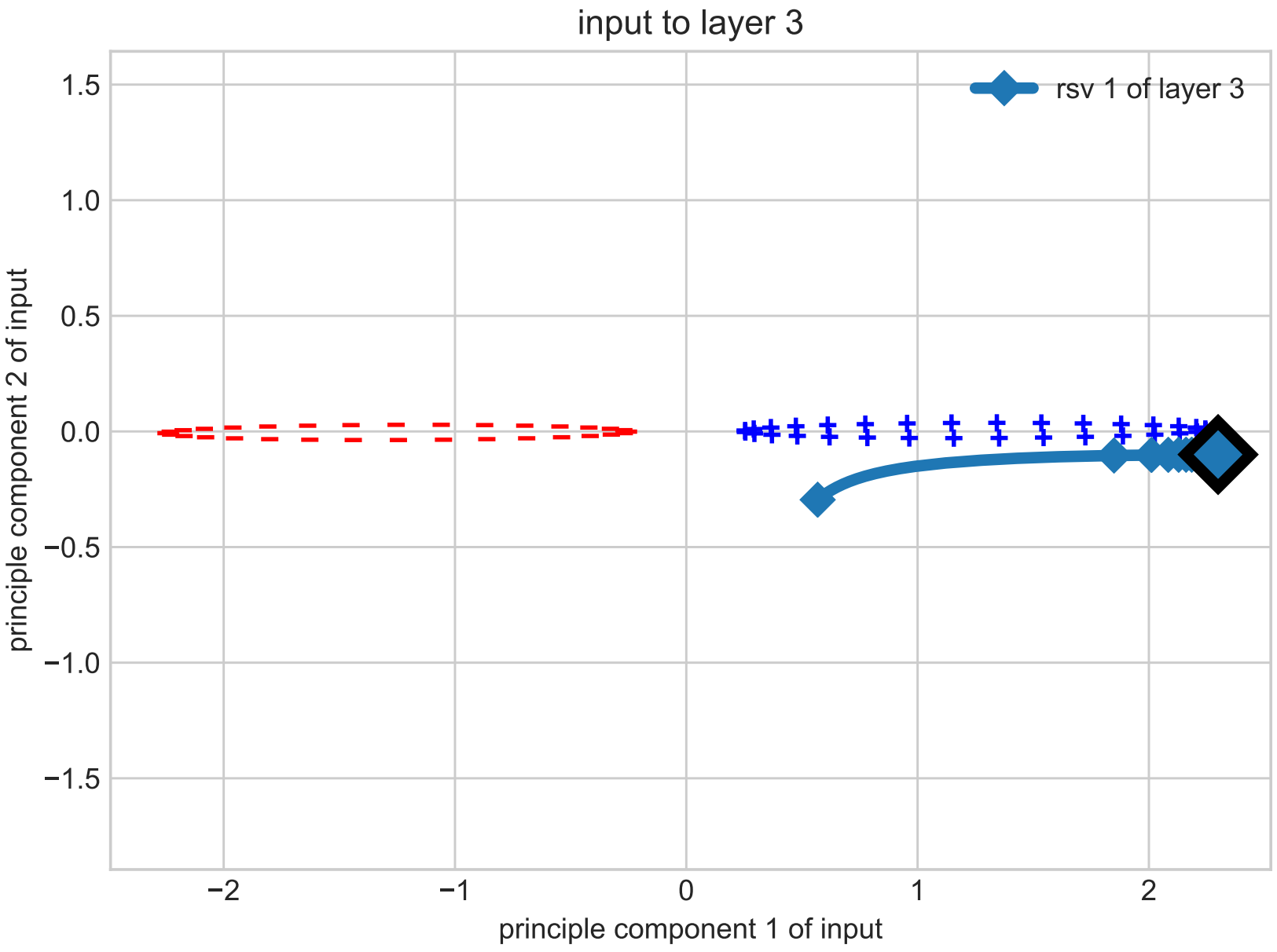

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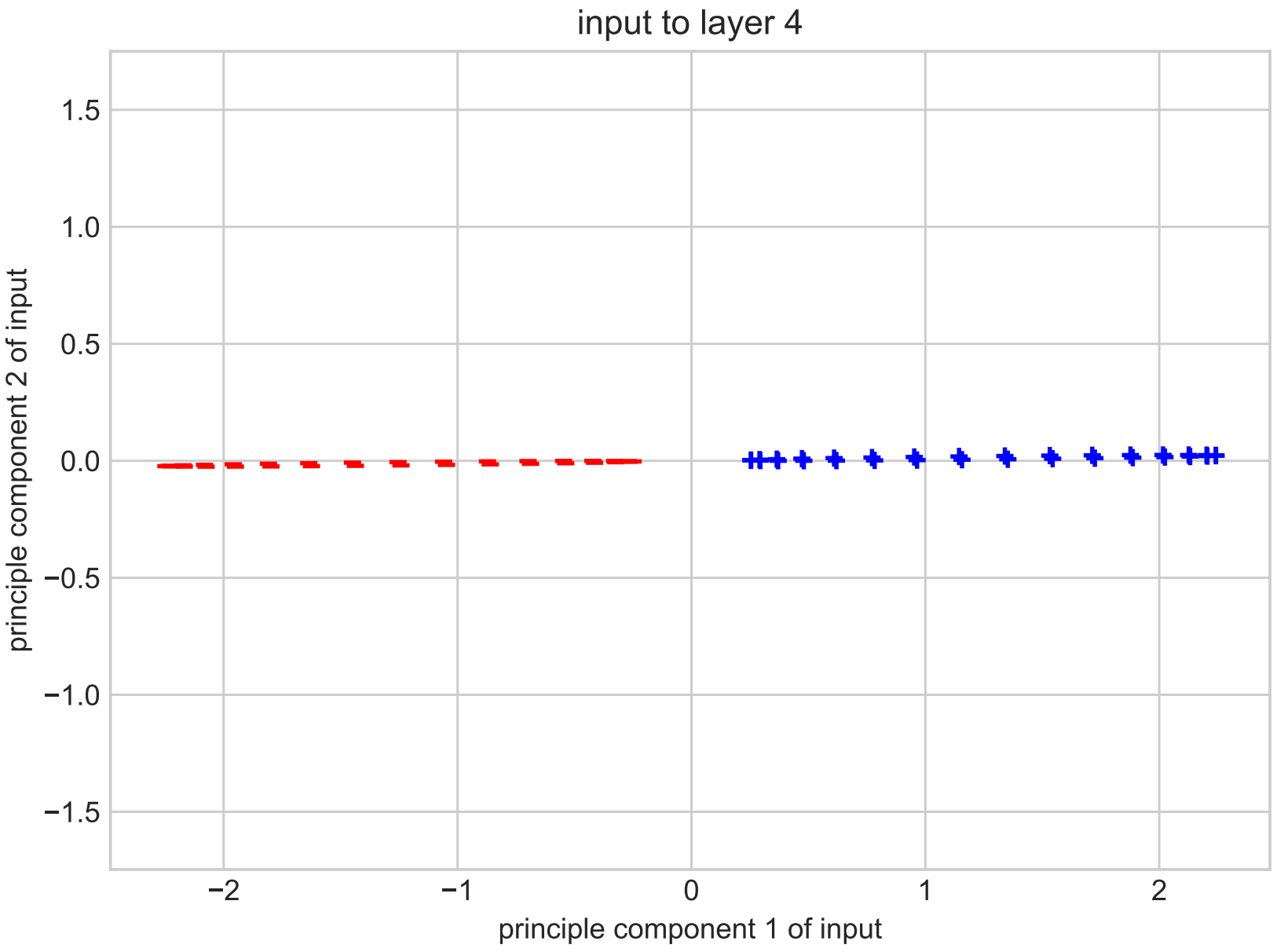

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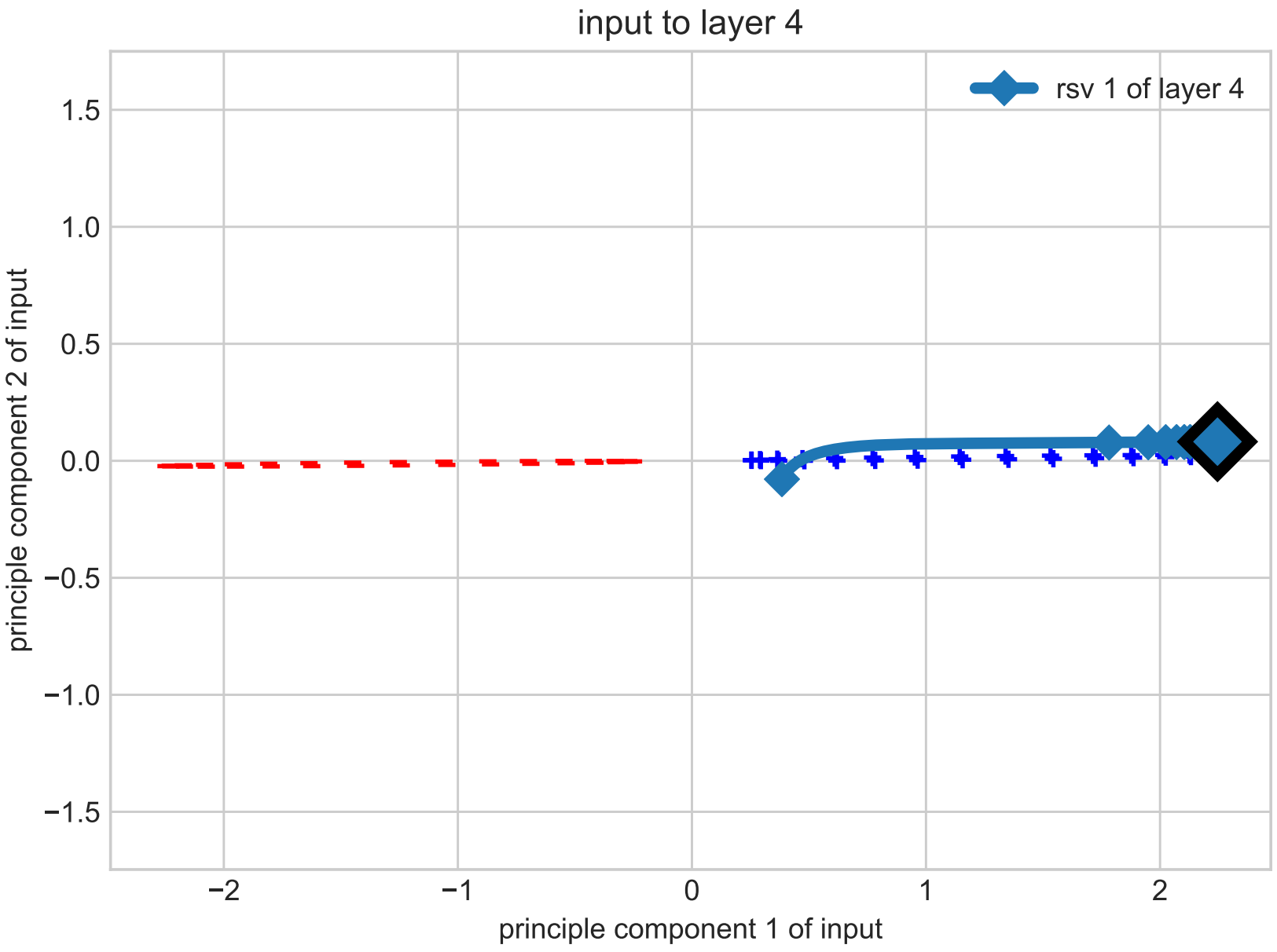

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Remarks.

- Related work with convolution layers (Gunasekar-Lee-Soudry-Srebro '18).
- Generalization consequence: not just margins, can shrink "nuisance term"!
- Empirically on ReLU networks, *some alignment occurs*: ratios $\|W_i\|_{\mathrm{F}}/\|W_i\|_2$ are small.

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Proof remarks.

- Never underestimate simply writing down the gradient!

$$-\frac{\mathrm{d}W_i}{\mathrm{d}t} = \frac{\mathrm{d}\widehat{\mathcal{R}}}{\mathrm{d}W_i} = W_{i+1}^{\mathsf{T}} \cdots W_L^{\mathsf{T}} \nabla \widehat{\mathcal{R}}(w_{\mathrm{prod}}) W_1^{\mathsf{T}} \cdots W_{i-1}^{\mathsf{T}}.$$

  Implies: gradients rank 1, and $W_i^{\mathsf{T}} \left(\frac{\mathrm{d}\widehat{\mathcal{R}}}{\mathrm{d}W_i}\right) = \left(\frac{\mathrm{d}\widehat{\mathcal{R}}}{\mathrm{d}W_{i-1}}\right) W_{i-1}^{\mathsf{T}}$ (Du et al., 2018; Arora et al, 2018; Folklore).

- Can use perceptron proof ideas!

One approach to nonlinearities:

NTK (neural tangent kernel).

- $f(x; w)$ denotes network output with params w, input x.
- Let $\ell_i'(w) := \ell'\left(f(x_i; w), y_i\right)$; gradient step has form

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- If $\eta \approx 0$, evolution of predictions is controlled by *kernel*

$$(x, x') \mapsto \nabla_w f(x; w)^\mathsf{T} \nabla_w f(x'; w).$$

The initial kernel

What if we replace $\nabla_w f(x; w)^\mathsf{T} \nabla_w f(x'; w)$ with $\mathbb{E}_{w_0} \nabla_w f(x; w_0)^\mathsf{T} \nabla_w f(x'; w_0)$?

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- Key question: does this relate to deep networks?

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  - High level reason: standard initialization means increasing width rescales function; risk surface becomes flat.
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- Unfortunately, these proofs require width $\Omega(n)$.
- Empirically:
  - True for initial iterations on standard architectures.
  - In some rare cases, explicit NTK can match or slightly outperform deep network (!).

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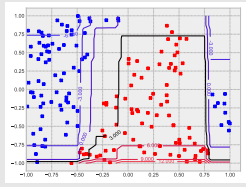
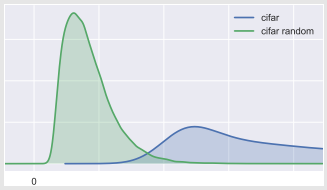
- NTK initial phase can still pick decent parameters; margin analysis can then say loss goes to 0 (Lyu-Li '19).
- These analyses require large width, kill generalization; preceding margin analysis doesn't guarantee sufficient margin.
- This analysis (and "mean field") are only ways I know to really take advantage of random initialization!



Margins.



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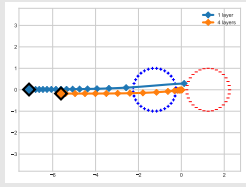

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- Optimization and generalization are still open.
- Margin theory was effective with boosting;
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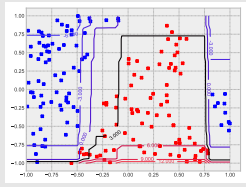
- Freezing the initial kernel ("NTK")
  does prove arbitrarily low training error in some nonlinear cases,
  but does not generalize.
  Moreover, it is known deep learning diverges from NTK,
  but only in limited constructions (AllenZhu-Li '19).



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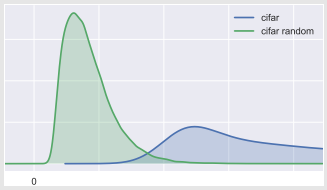

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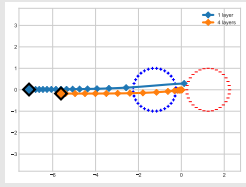

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