Deep Learning (BEV033DLE)
Lecture 7. Regularization

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Regularization Methods

✦ **Problem: Overfitting to a Finite Training Data**

- Can classify the training data with 100% accuracy
- Test error is substantially larger than training error

✦ **Explicit Regularization:**

- Parameter Regularization (L_1, L_2, general norms)
- Data Augmentation (random transforms, noises)
- Injected Noises (Dropout)

✦ **Implicit Regularization (Inductive Bias):**

- Network Architecture (activations, structure, normalization, attention)
- Initialization, SGD dynamics, Batch Normalization
- Loss function, task formulation, transfer learning

Parameter Regularization

General Setup

- Regularized training objective:

$$\min_\theta \mathcal{L}(\theta) + \lambda R(\theta) = \min_\theta \sum_i l_i(\theta) + \lambda R(\theta)$$

  - $l_i(\theta)$ - loss function for the data point (x_i, y_i)
  - $R(\theta)$ - function not depending on data
  - λ - regularization strength

- Can be interpreted as maximum a posteriori (MAP) parameter estimation:
  - $p(D|\theta)$ - likelihood of the data given parameters
  - $p(\theta) \propto \exp(-\lambda R(\theta))$ - prior on the model parameters
  - $p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)}$ - Bayesian posterior over parameters
  - $\hat{\theta}_{\text{MAP}} = \operatorname*{argmax}_\theta p(D|\theta)p(\theta) = \operatorname*{argmax}_\theta \log p(D|\theta) + \log p(\theta)$

  [RPZ lecture 3:(Parameter Estimation: Maximum a Posteriori (MAP))]

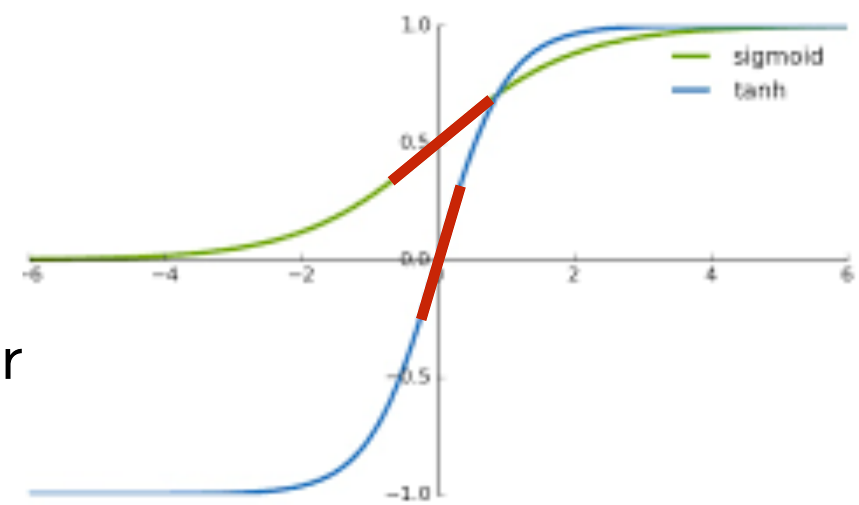
- In practice also commonly appears in the form independent of the amount of data:

$$\min_\theta \frac{1}{n} \sum_i l_i(\theta) + \lambda R(\theta)$$

  - λ is tuned for a given dataset with cross-validation

L_2 Regularization

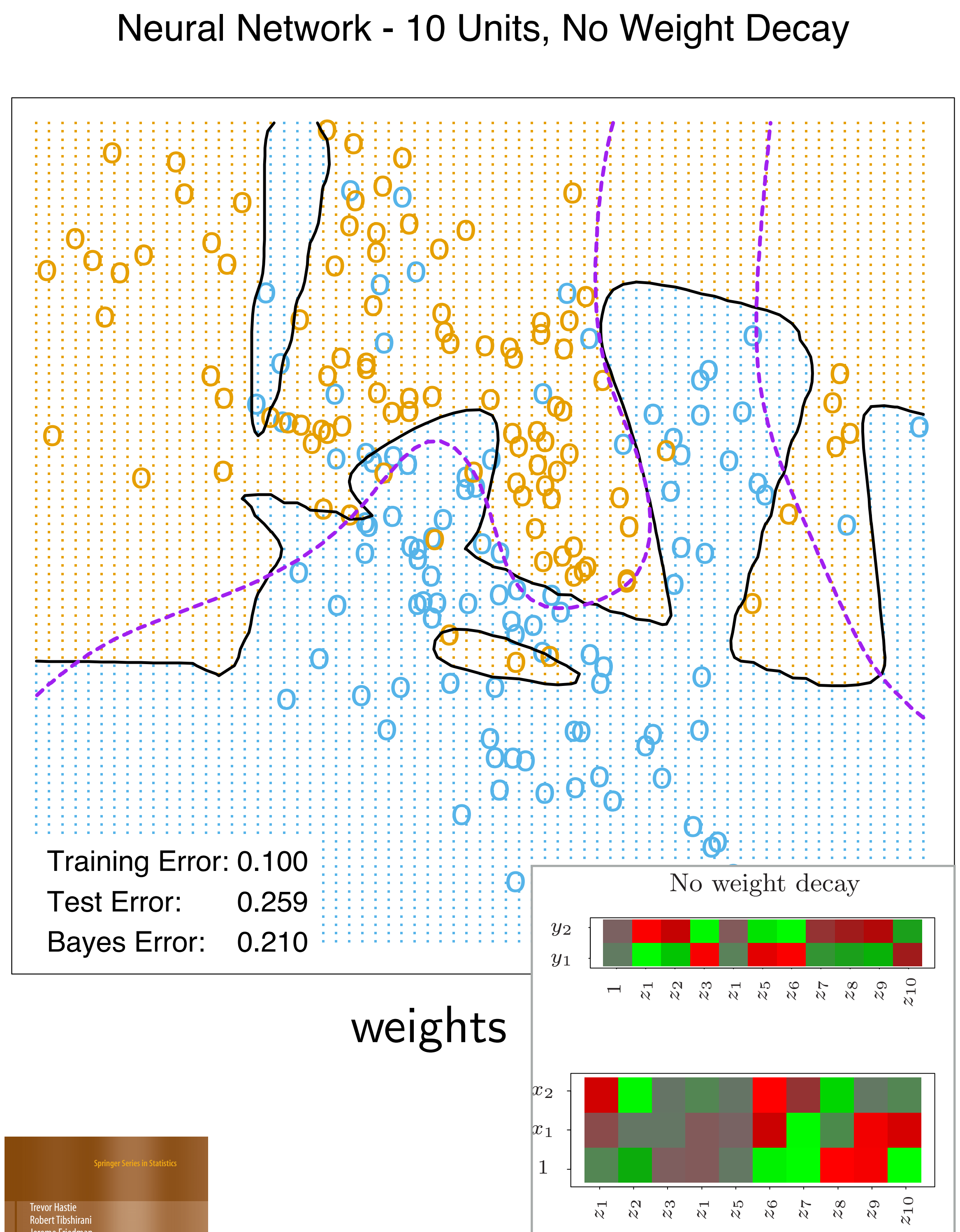
- L_2-regularization: $R(\theta) = \frac{1}{2}\|\theta\|^2$
- **Linear Regression**:
  - Ridge regression: $\min_{\theta} \sum_i (\theta^\top x_i - y_i)^2 + \frac{\lambda}{2}\|\theta\|^2$
  - Solution: $\hat{\theta} = (XX^\top + \lambda I)^{-1} X^\top y$
  - Equivalent to *multiplicative noise* on inputs: $\min_\theta \mathbb{E}_{\xi \sim \mathcal{N}(\mathbf{1}, \lambda^2 I)} \sum_i (\langle \theta, \xi \odot x_i \rangle - y_i)^2$
  - Even small λ helps with underdetermined problems
- **Linear Classifiers**:
  - SVMs maximize margin $\frac{1}{\|w\|}$ by minimizing $\|w\|^2$ under constrains
  - Generalization guarantees improve with larger margin



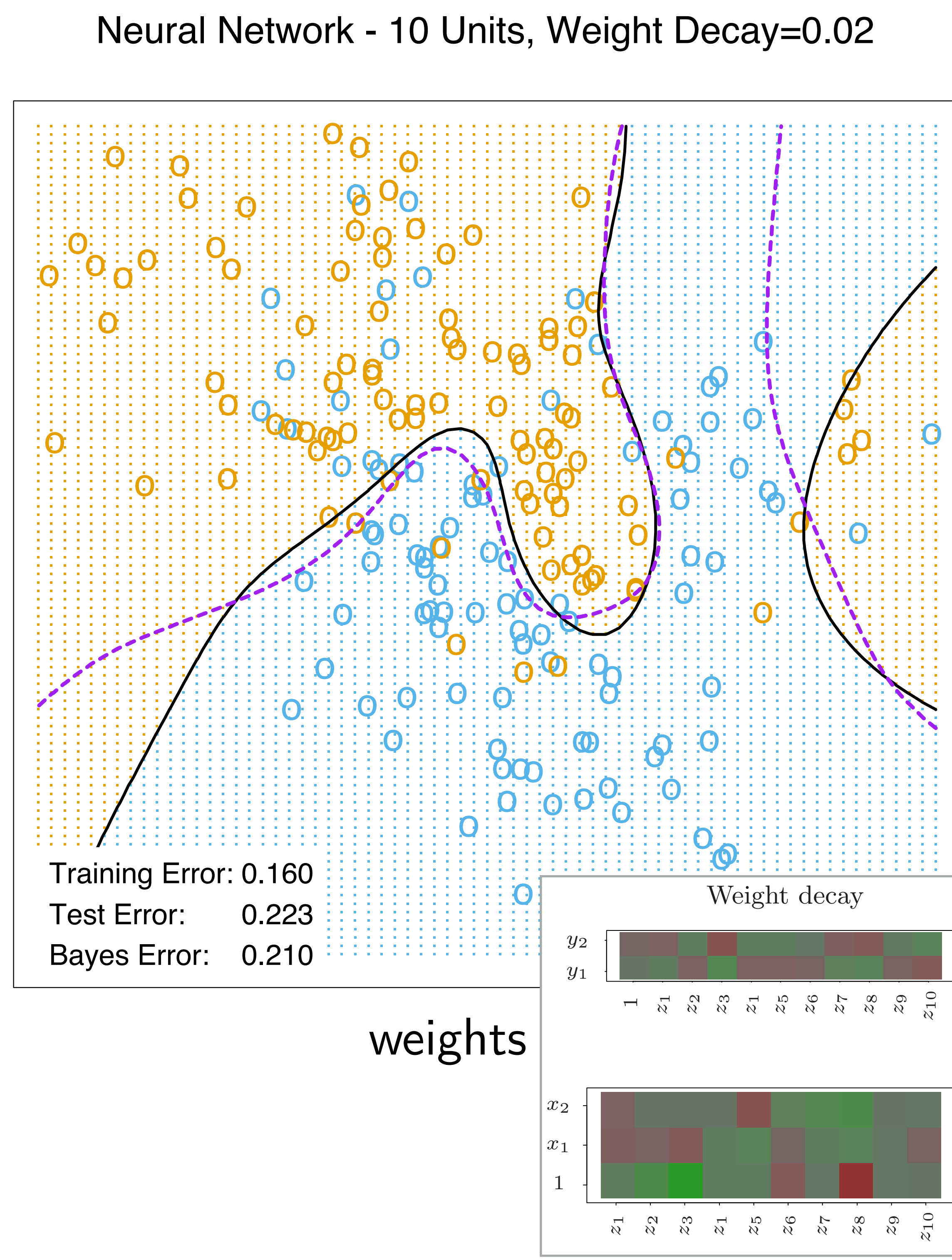
- **Sigmoid NNs**:
  - Small $\|\theta\| \Rightarrow$ sigmoid outputs are close to linear

    $\Rightarrow$ smoother classification boundary

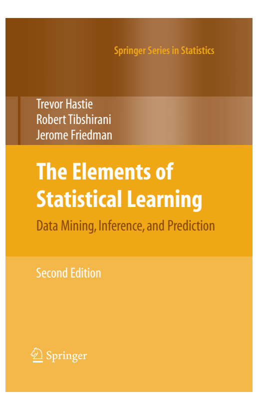
L_2 Regularization: Simulated Data Example



weights



weights

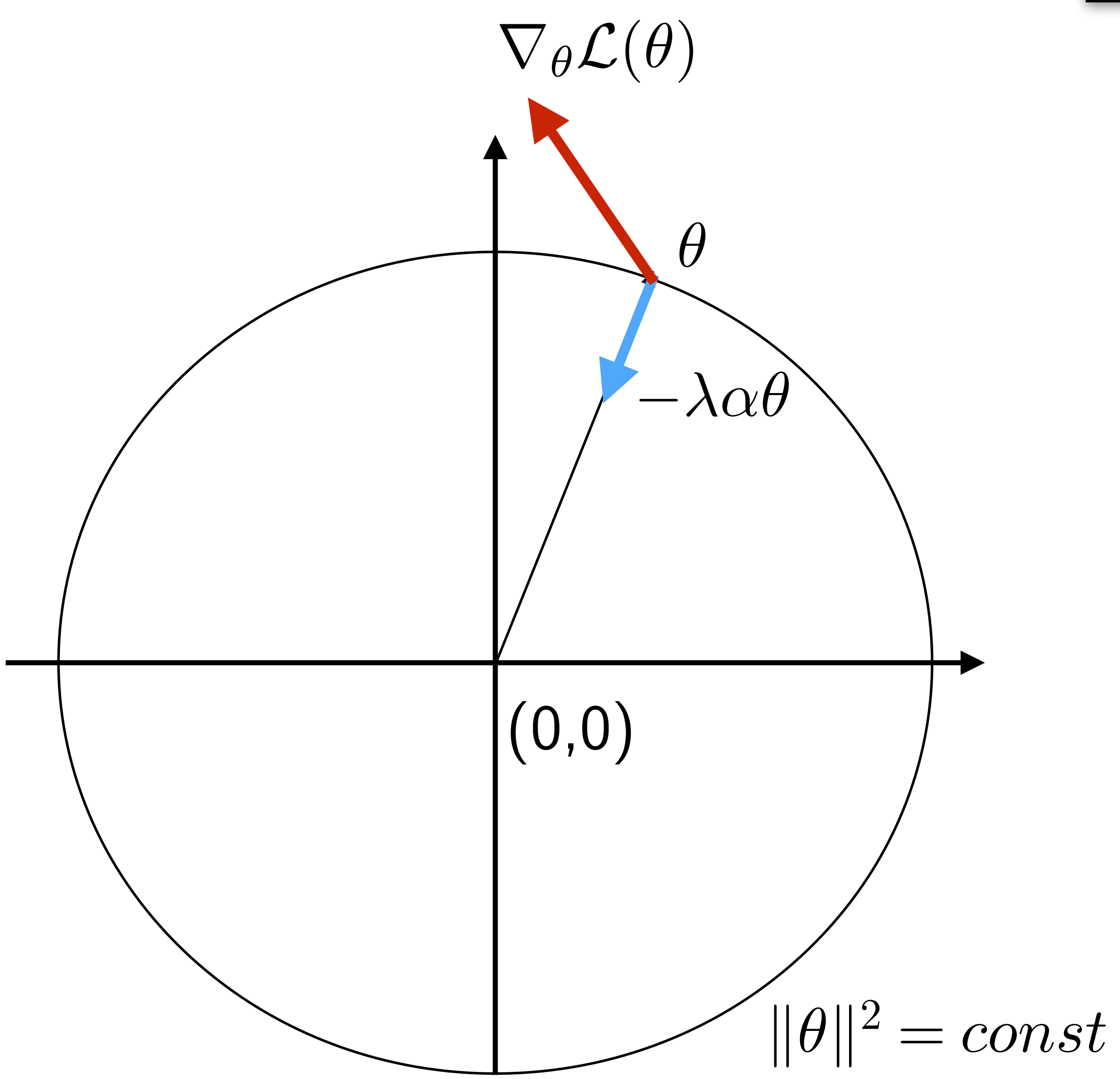


Hastie, Tibshirani and Friedman: The Elements of Statistical Learning

https://web.stanford.edu/~hastie/ElemStatLearn/

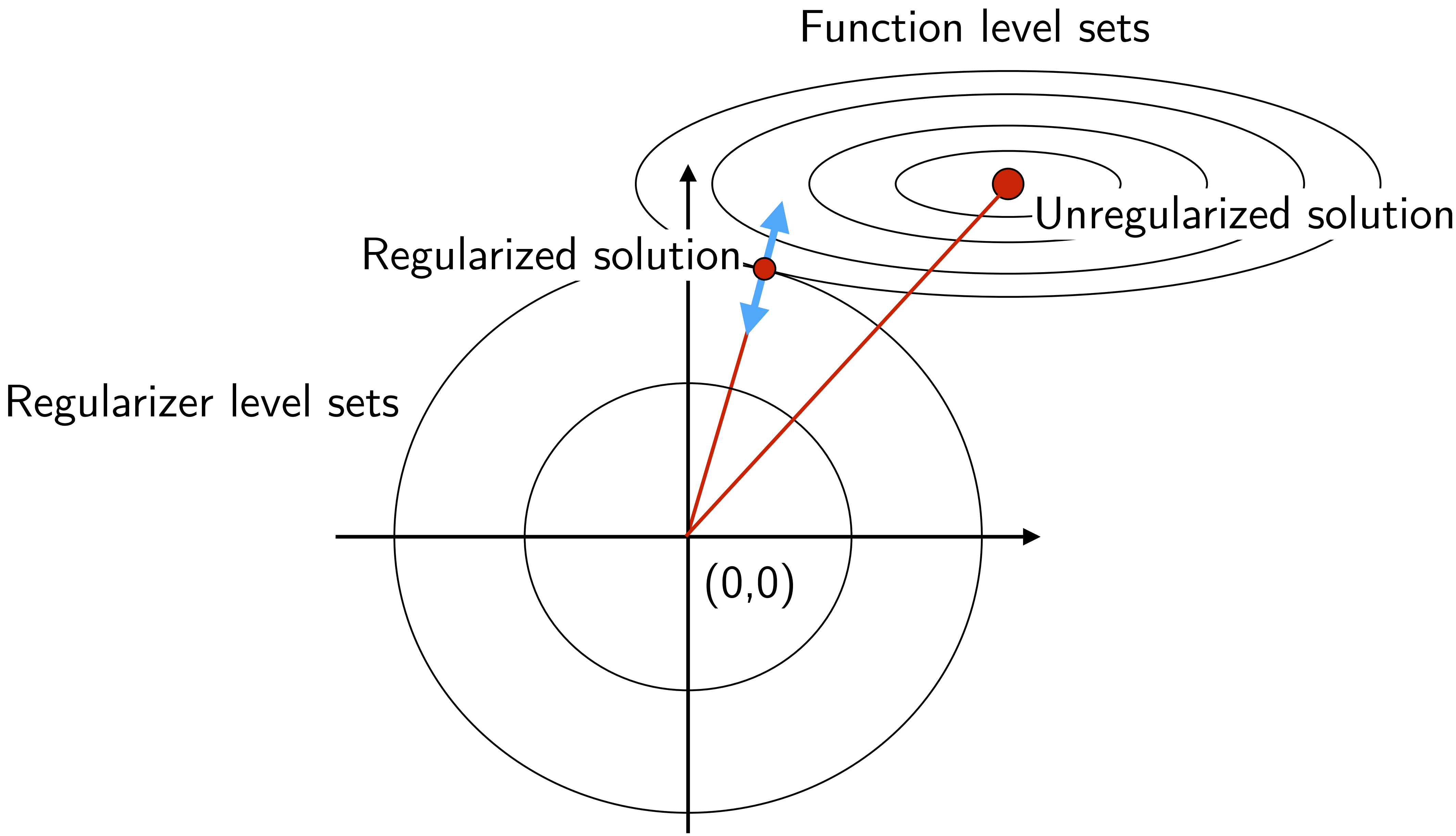
L_2 Regularization: Weight Decay

- $\min_{\theta} \mathcal{L}(\theta) + \frac{\lambda}{2}\|\theta\|^2$
- Gradient descent:
  - $g^t := \nabla_\theta \mathcal{L}(\theta) + \lambda\theta$
  - $\theta^{t+1} = \theta^t - \alpha g^t$
  - $\theta^{t+1} = \underbrace{(1-\alpha\lambda)}_{\text{decay}}\theta^t - \alpha\nabla_\theta\mathcal{L}(\theta)$



- In neural networks:
  - There is typically a manifold of optimal solutions, small regularization of order 10^{-5} may have effect

L2 Regularization

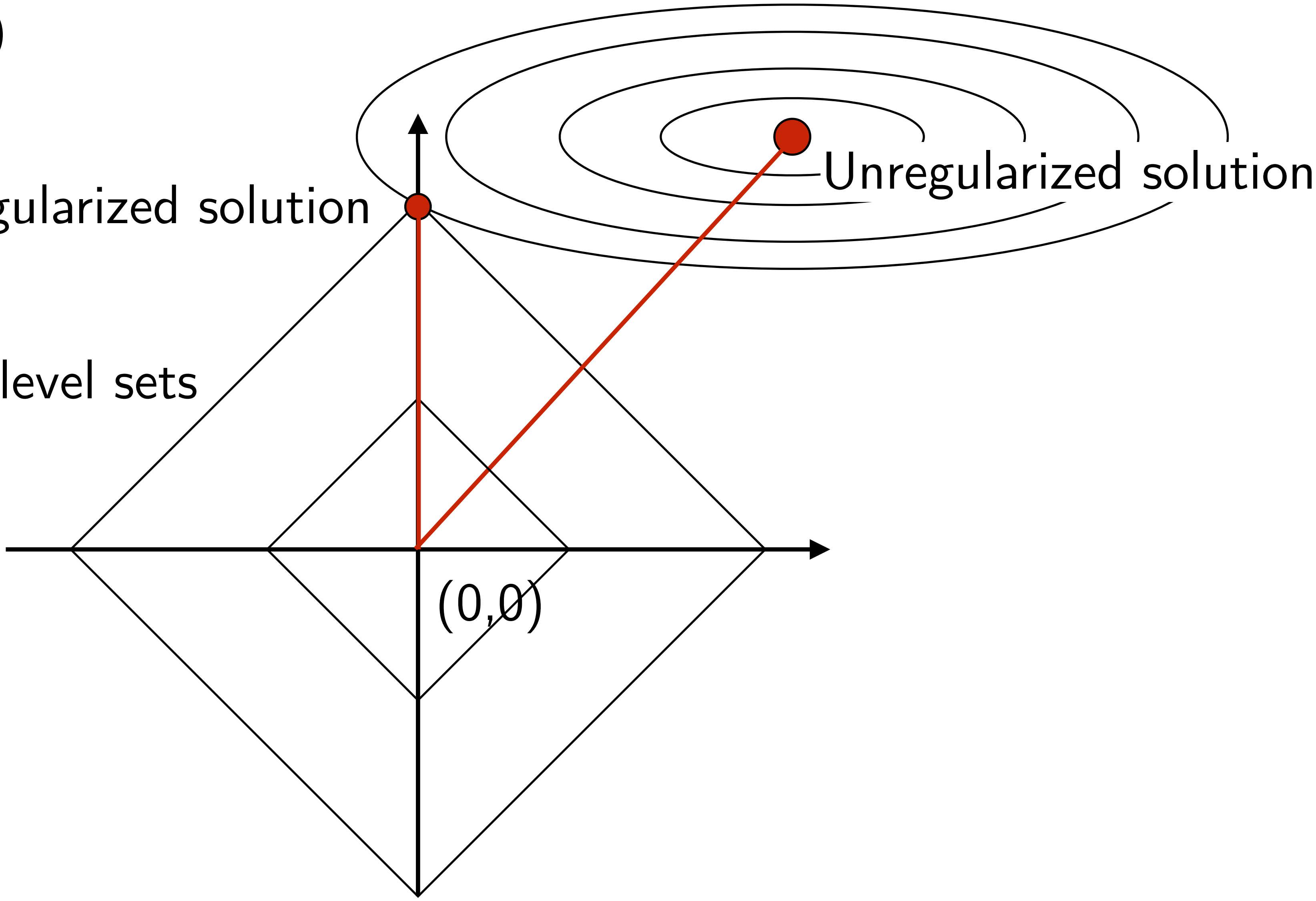


- L_2 regularization effect (approximately quadratic loss):
  - Parameter shrink along eigenvectors of the loss Hessian by $\frac{s_i}{s_i+\lambda}$
  - s_i – eigenvalue, curvature along i'th eigenvector

L1 Regularization

- $R(\theta) = \|\theta\|_1 = \sum_k |\theta_k|$

  $\nabla R(\theta) = \text{sign}(\theta)$



- L1 regularization effect:
  - promotes sparsity
  - for better generalization we typically do not want sparsity (= less parameters)

L_p Regularization -- Max p-Margin

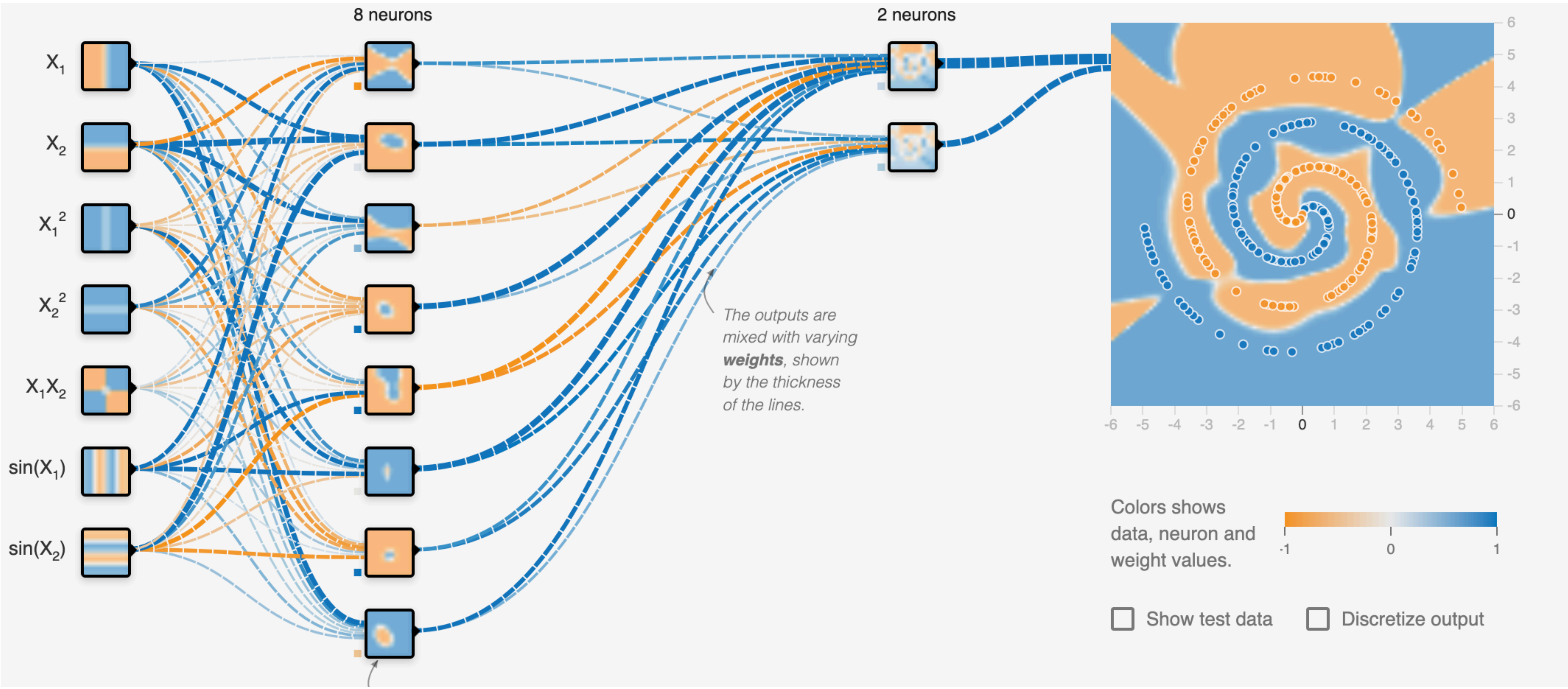
- **Binary classification**
  - Training set $\{x_i, y_i\}_{i=1}^N$ with $y_i \in \{1, -1\}$.
- **Linear predictor**
  - Score: $s(x) = w^\mathsf{T}\phi(x)$,
  - Decision: $y = \mathrm{sign}(s)$,
  - Regularized loss solution $w^*(\lambda) = \arg\min_w \sum_i l(y_i s(x_i)) + \lambda \|w\|_p^p$.
- **Theorem** [Rosset et al. 2003]:
  - Assume that data is linear separable and l is monotone and decreasing "quickly" (includes SVM hinge loss, logistic regression loss, AdaBoost exponential loss).
  - Then

$$\lim_{\lambda \to 0} \|w^*(\lambda)\|_p = \infty,$$

$$\lim_{\lambda \to 0} \frac{w^*(\lambda)}{\|w^*(\lambda)\|_p} = w^M,$$

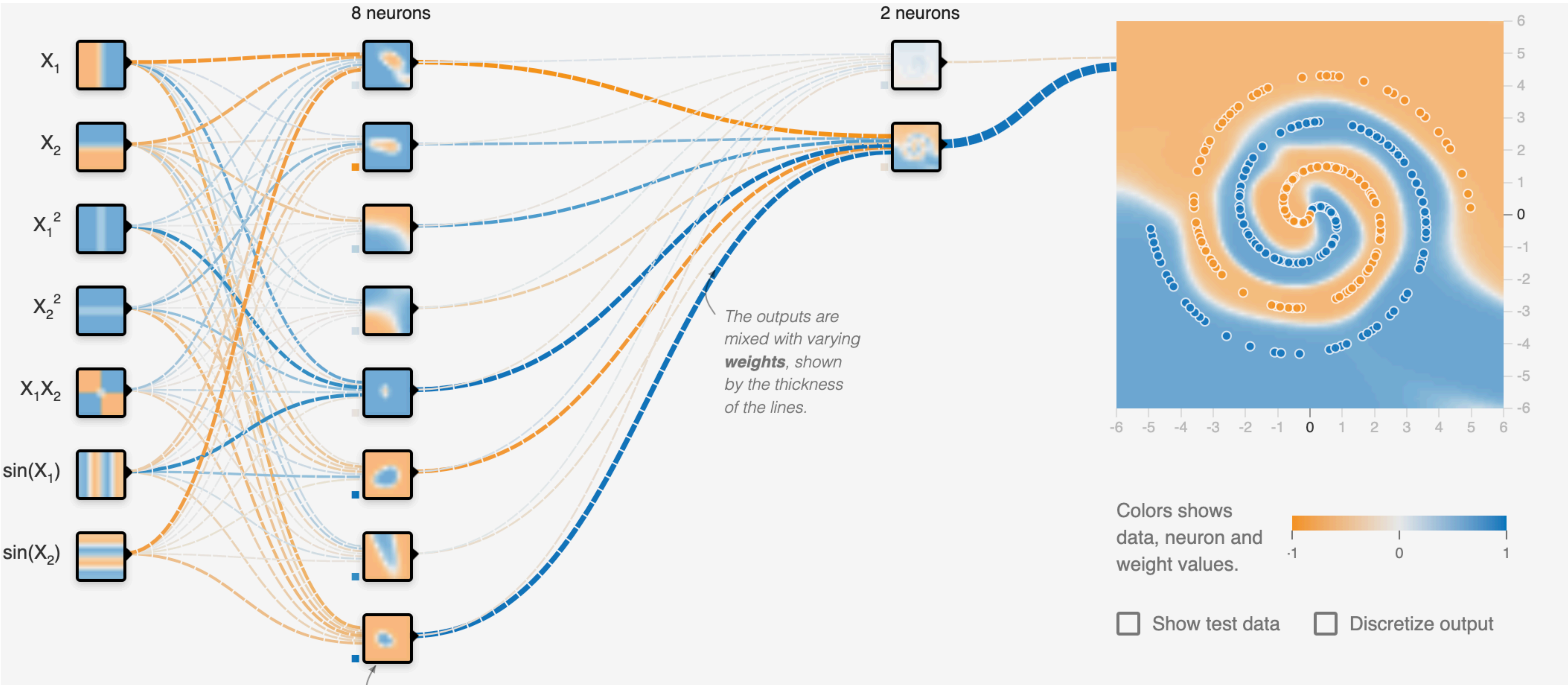
where $w^M = \arg\max_{\|w\|_p = 1} \min_i y_i w^\mathsf{T}\phi(x)$ is the max-margin separating hyperplane.

Example: No regularization

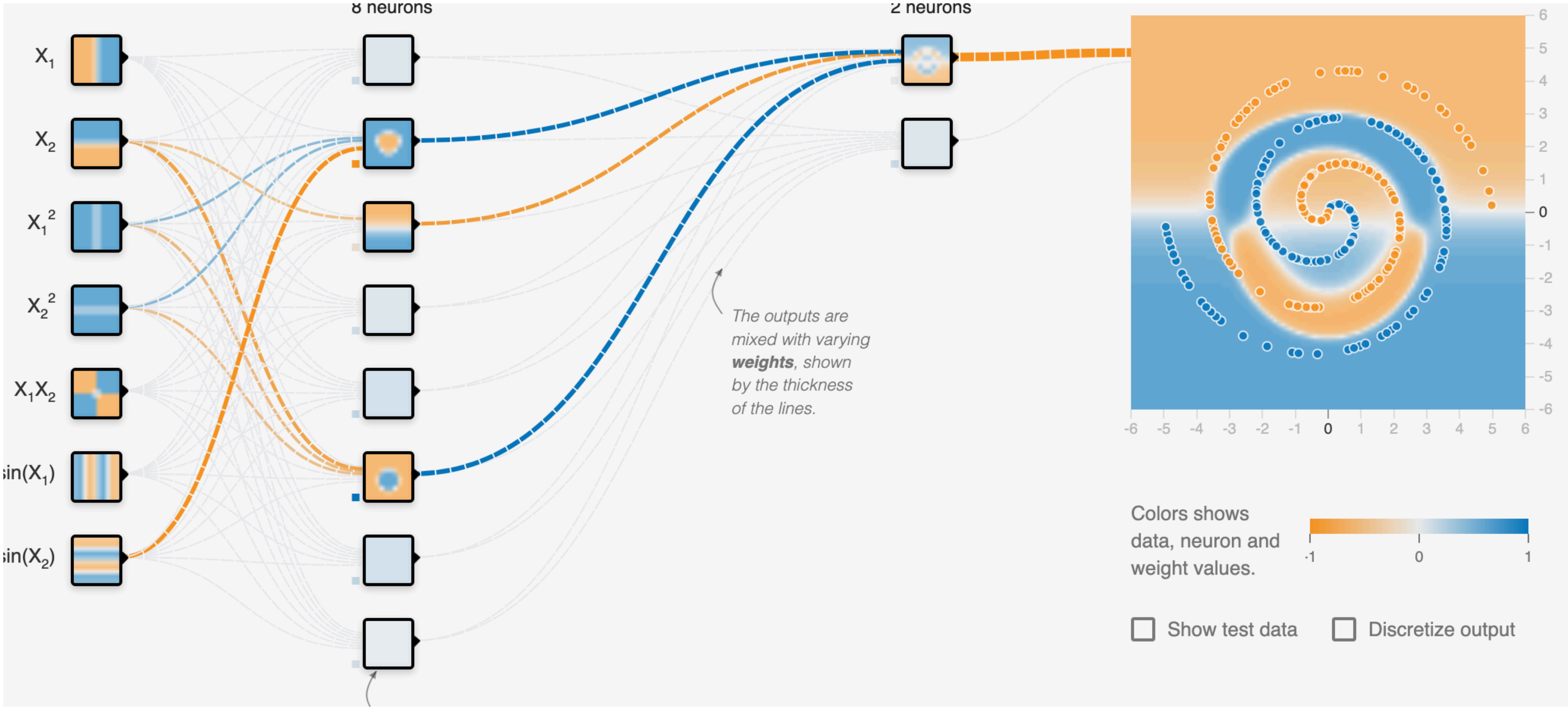


[Tensorfolw playground]

Example: L_2 Regularization

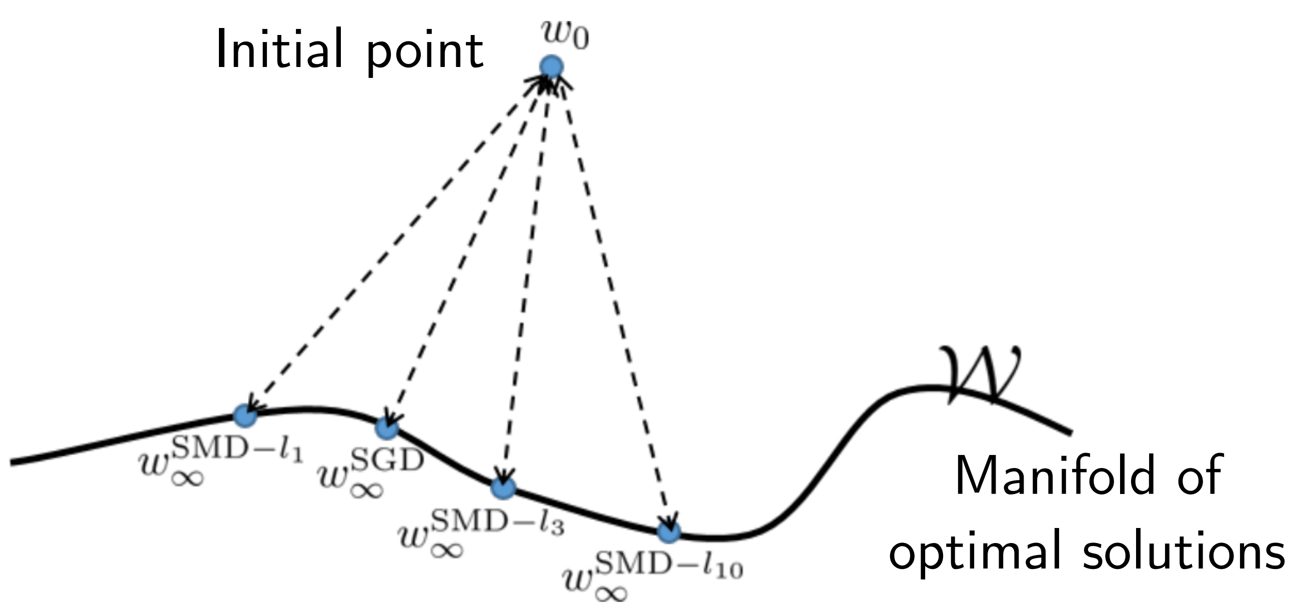


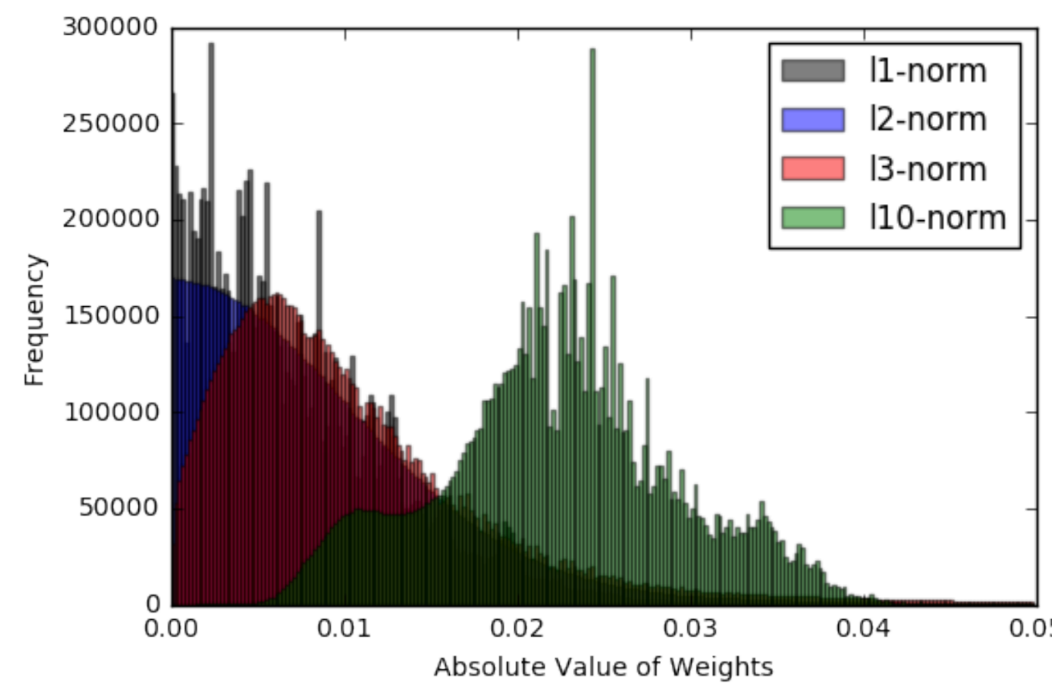
Example: L_1 Regularization



Implicit Regularization by p-Norm-Steppest SGD

- Consider step proximal problem: $\min_x \langle \nabla f(x_0), x - x_0 \rangle + \lambda \|x - x_0\|_p^p$
  - i.e., p-norm SGD (mirror descent)
- Using different p leads to solutions with different properties

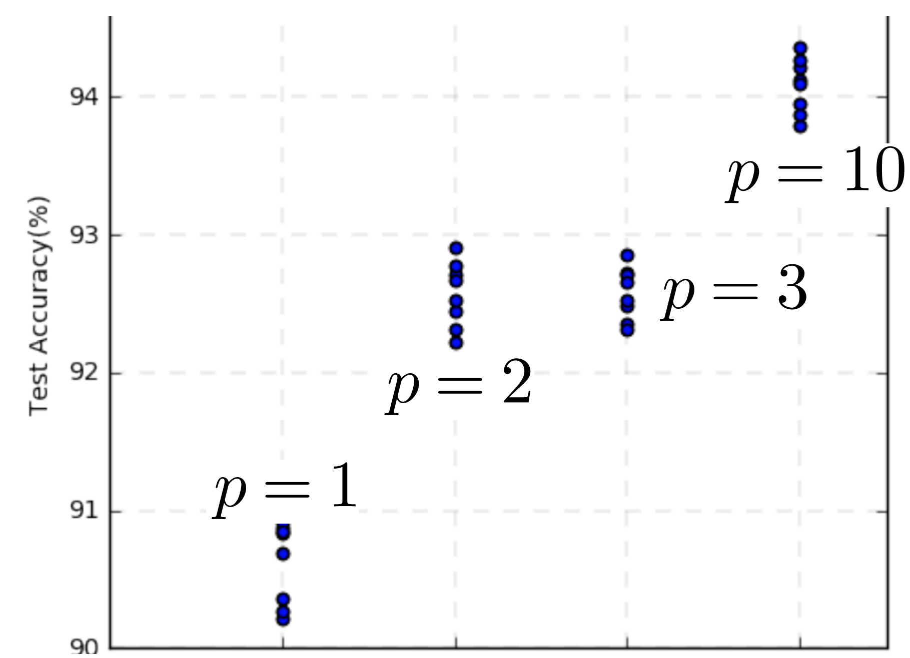




- Iterates tend to $\mathrm{argmin}_{w \in \mathcal{W}} \|w - w_0\|_p^p$, the closest point in the respective norm

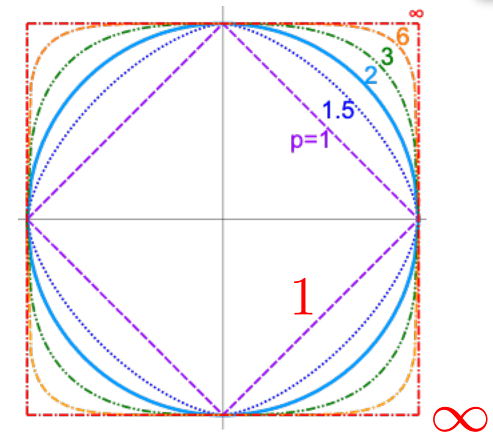
	SMD 1-norm	SMD 2-norm (SGD)	SMD 3-norm	SMD 10-norm
1-norm BD	141	9.19×10^3	4.1×10^4	2.34×10^5
2-norm BD	3.15×10^3	562	1.24×10^3	6.89×10^3
3-norm BD	4.31×10^4	107	53.5	1.85×10^2
10-norm BD	6.83×10^{13}	972	7.91×10^{-5}	2.72×10^{-8}

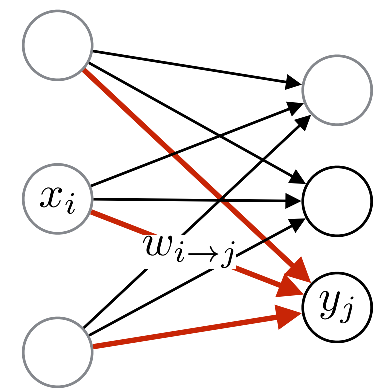
- Different sparsity and generalization



[Azizan et al. (2022):
Stochastic Mirror Descent on Overparameterized Nonlinear Models]

★ Group Norm, Generalization Bounds





- **More General Norms**:
  - L_p norm: $\|\theta\|_p = \left(\sum_i |\theta_i|^p\right)^{\frac{1}{p}}$
  - $p < 1$ is closer to counting non-zero weights, *i.e.* sparsity
  - $p = \infty$ results in $R(\theta) = \max_i \theta_i$
  - Hidden layer: $y_j = \sum_i w_{i\to j} x_i$
  - $L_{p,q}$ norm: $\|W\|_{p,q} = \left(\sum_j \left(\sum_i |w_{i\to j}|^p\right)^{\frac{q}{p}}\right)^{\frac{1}{q}}$

- **Generalization Bounds**:
  - Feed-forward NN with L layers, ReLU activations and weights W^k, $k = 1 \dots L$.
  - Class of predictors $\mathcal{F}$ defined by $\prod_{k=1}^{L} \|W^k\|_{p,q} \leq \psi$ for $q, p > 1$.
  - **Theorem** [Neyshabur 2017] For any $\delta > 0$ with probability $1 - \delta$ over draws of training set $\mathcal{T}$ of size N:

0-1 Risk

Training risk on $\mathcal{T}$ with margin γ

Radamacher complexity of linear class $\propto \sqrt{\frac{1}{N}}$

$$R \leq \hat{R}_{\mathcal{T},\gamma} + \psi \frac{1}{\gamma} 2^L \left(H^{(L-1)\max(1-\frac{1}{p}-\frac{1}{q},0)}\right) C^{\text{linear}}_{N,p,n_{in}} + \sqrt{\frac{8ln(2/\delta)}{N}}$$

Number of neurons

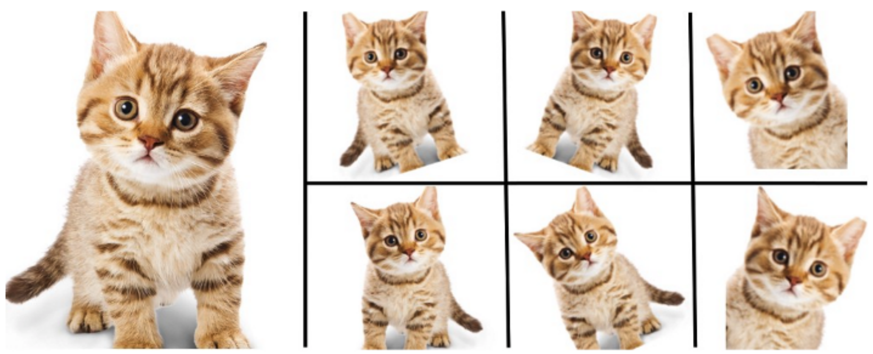
Vanishes when $q \leq \frac{p}{p-1}$

Data Augmentation

Data Augmentation (Image Classification)

✦ Random transforms:

- the transformed input should be as likely in the data distribution
- the class label should stay the same
- original image should be kept with sufficient probability



Geometric: scale, crop, rotation, non-rigid

Photometric: brightness, contrast

Filters: blur, sharpen, low-pass

Simulation: acquisition noise, fully synthetic

✦ Pros:

- Can improve generalization
- Can improve model robustness / enforce invariances of features

✦ Cons:

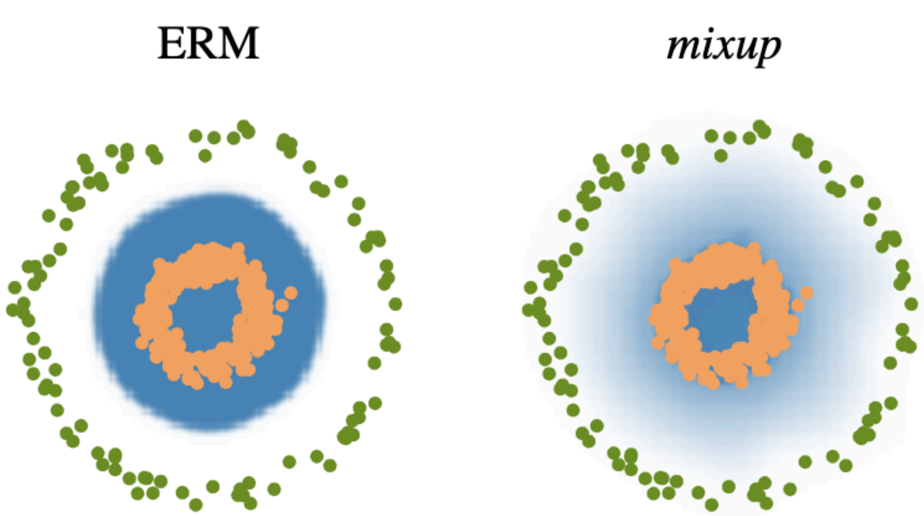
- altering the true data distribution too much could worsen performance (e.g. too much noise, synthetic-real gap)
- increases training time

Data Augmentation (Image Classification)

✦ **Mixup** (Zhang et al .2018):

$$\tilde{x} = \lambda x_i + (1-\lambda) x_j, \qquad \text{where } x_i, x_j \text{ are raw input vectors}$$
$$\tilde{y} = \lambda y_i + (1-\lambda) y_j, \qquad \text{where } y_i, y_j \text{ are one-hot label encodings}$$

Inductive bias towards linear predictors -- smoother confidences and decision boundaries



Dataset	Model	ERM	*mixup*
CIFAR-10	PreAct ResNet-18	5.6	**4.2**
	WideResNet-28-10	3.8	**2.7**
	DenseNet-BC-190	3.7	**2.7**
CIFAR-100	PreAct ResNet-18	25.6	**21.1**
	WideResNet-28-10	19.4	**17.5**
	DenseNet-BC-190	19.0	**16.8**

Powerful idea to augment an image: use other images (labelled or not)

($\star$) Cross-entropy is linear in the target $y \Rightarrow$ reduces to regular data augmentation

Injected Noises / Dropout

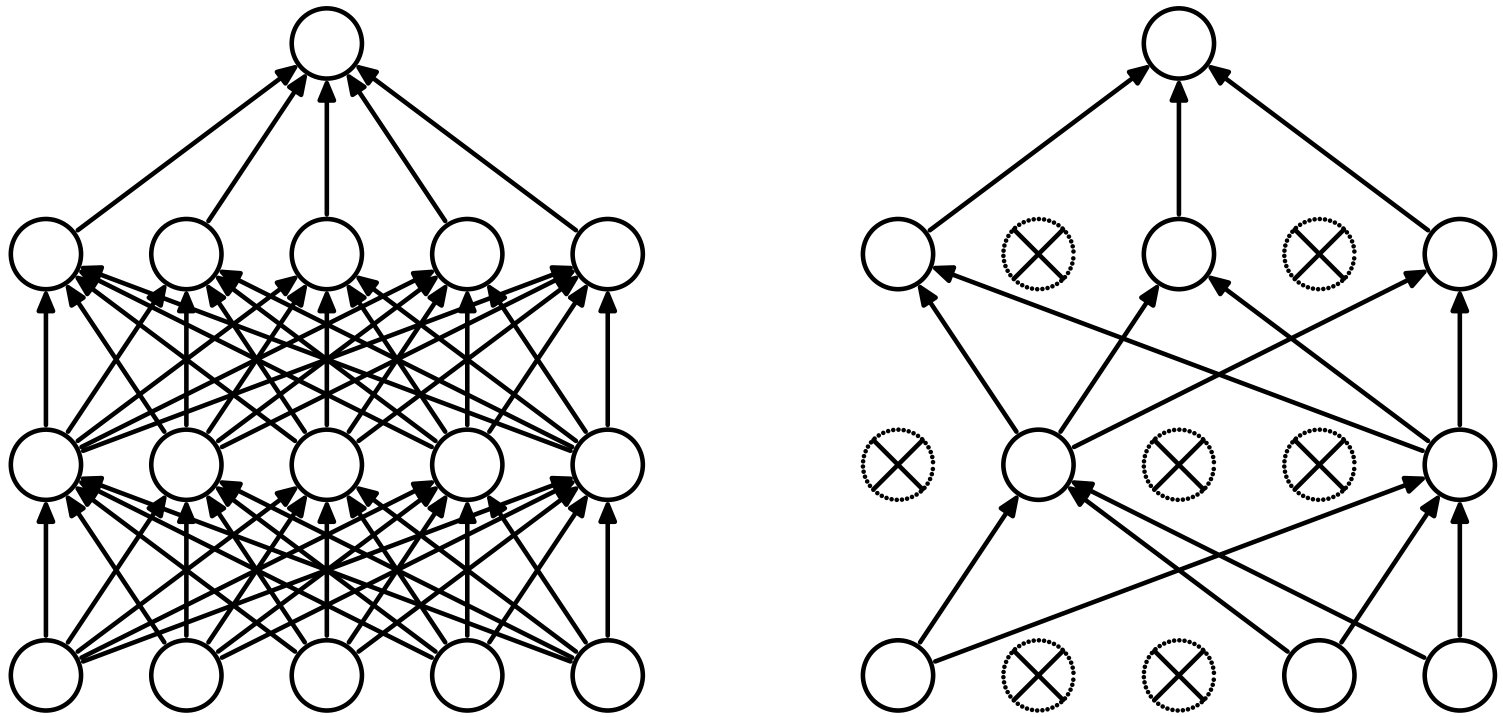
✦ **Injected Noises:**

- input
- deep features
- parameters
- gradient updates

| Bayesian learning, robust local minima

(The last line refers to "parameters" and "gradient updates".)

Dropout



(a) Standard Neural Net (b) After applying dropout.

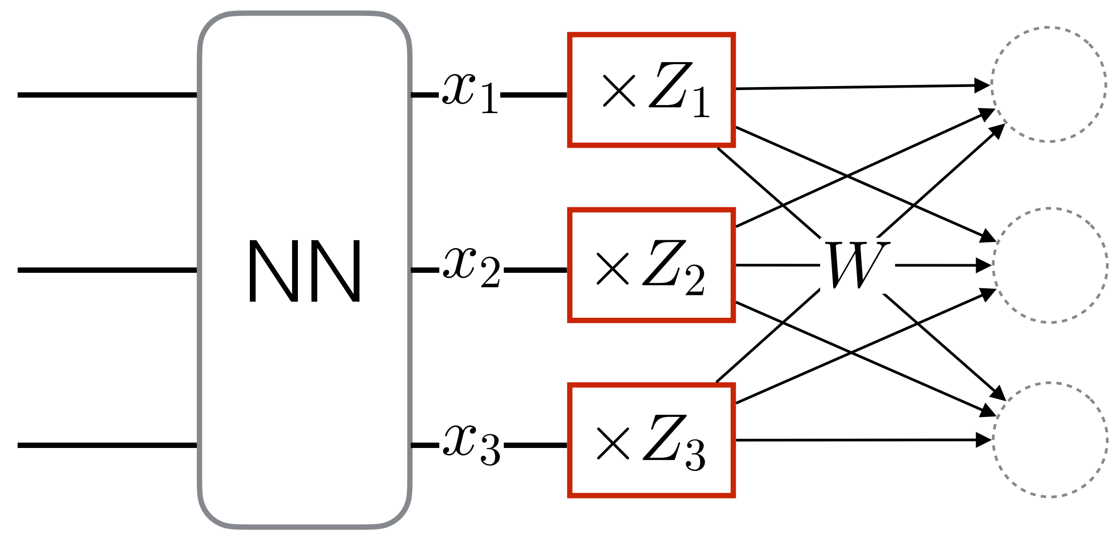
[Hinton et al. (2012) Improving neural networks by preventing co-adaptation of feature detectors]

[Srivastava et al. (2014) Dropout: A Simple Way to Prevent Neural Networks from Overfitting]

- During training:
  - Randomly, "drop" some neurons -- set their outputs to zero
  - This results in the associated weights not being used and we obtain a (random) subnetwork
  - When learning, the network develops robustness to units being dropped
- During testing:
  - Use all units -- approximates ensemble of all random subnetworks

Mathematical Model

- What does it mean mathematically?
  - Introduce random Bernoulli variables $Z_i = \begin{cases} 1, & \text{with probability } p, \\ 0, & \text{with probability } 1-p, \end{cases}$ multiplying outputs of the preceding layer
  - Can interpret outputs multiplied with 0 as dropped
  - Drop probability $q = 1 - p$
  - Next layer activations: $a = W(x \odot Z)$



$Z_i \sim$ Bernoulli(0.3)

- Prediction is random now?
  - Denote the network output as $f(x, Z; \theta)$
  - We have two choices how to make predictions:
    - **Randomized predictor:** $p(y|x, Z) = f(x, Z; \theta)$
    - **Ensemble:** $p(y|x) = \mathbb{E}_Z[f(x, Z; \theta)] = \sum_z p(z) f(x, z; \theta)$
- We use randomized predictor for training (easier)
- We use ensemble (or its approximation) for testing

Note: Gaussian multiplicative $\mathcal{N}(1, \sigma^2)$ noises work as well (Gaussian Dropout)

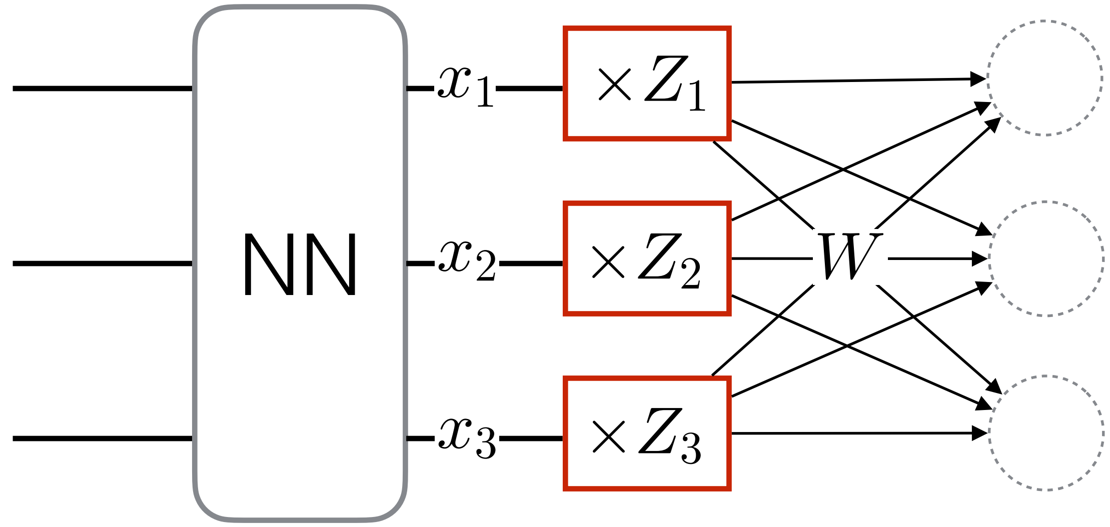
Training

- Expected loss of randomized predictor:
  - Double expectation in noises and data: $\mathbb{E}_Z\Big[\mathbb{E}_{(x,y)\sim\text{data}}\Big[l(y, f(x, Z; \theta))\Big]\Big]$
  - Same as: $\mathbb{E}_{Z\sim\text{Bernoulli}(q),\ (x,y)\sim\text{data}}\Big[l(y, f(x, Z; \theta))\Big]$
- What it means practically:
  - Draw a batch of data
  - For each data point i independently sample noises z_i
  - Unbiased loss estimate using a batch of size M:
    $\frac{1}{M}\sum_{i=1}^{M} l(y_i, f(x_i, z_i; \theta))$
  - Compute forward and backward pass
  - Will have increased variance of the stochastic gradient

Testing

- Use approximation (common default):
  - $\mathbb{E}_Z\Big[f(x,Z;\theta)\Big] \approx f(x, \mathbb{E}_Z[Z];\theta)$
  - Since $\mathbb{E}_Z[Z] = p$, we have

    $a = W(x \odot \mathbb{E}[Z]) = (pW)x$
  - i.e. need to scale down the weights



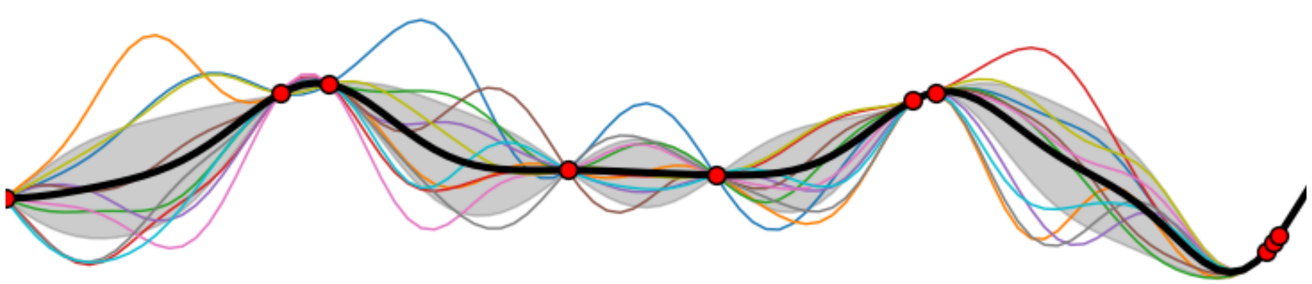
$Z_i \sim$ Bernoulli(0.3)

$E[Z] = p$

- Use sampling:
  - $\mathbb{E}_Z\Big[f(x,Z;\theta)\Big] \approx \frac{1}{M}\sum_{i=1}^{M} f(x_i, z_i;\theta)$
  - Generalizes slightly better than the above
  - Can be used to also estimate model uncertainty

- Both variants achieve a "committee" or "ensembling" effect

averaging of many well fitting models:

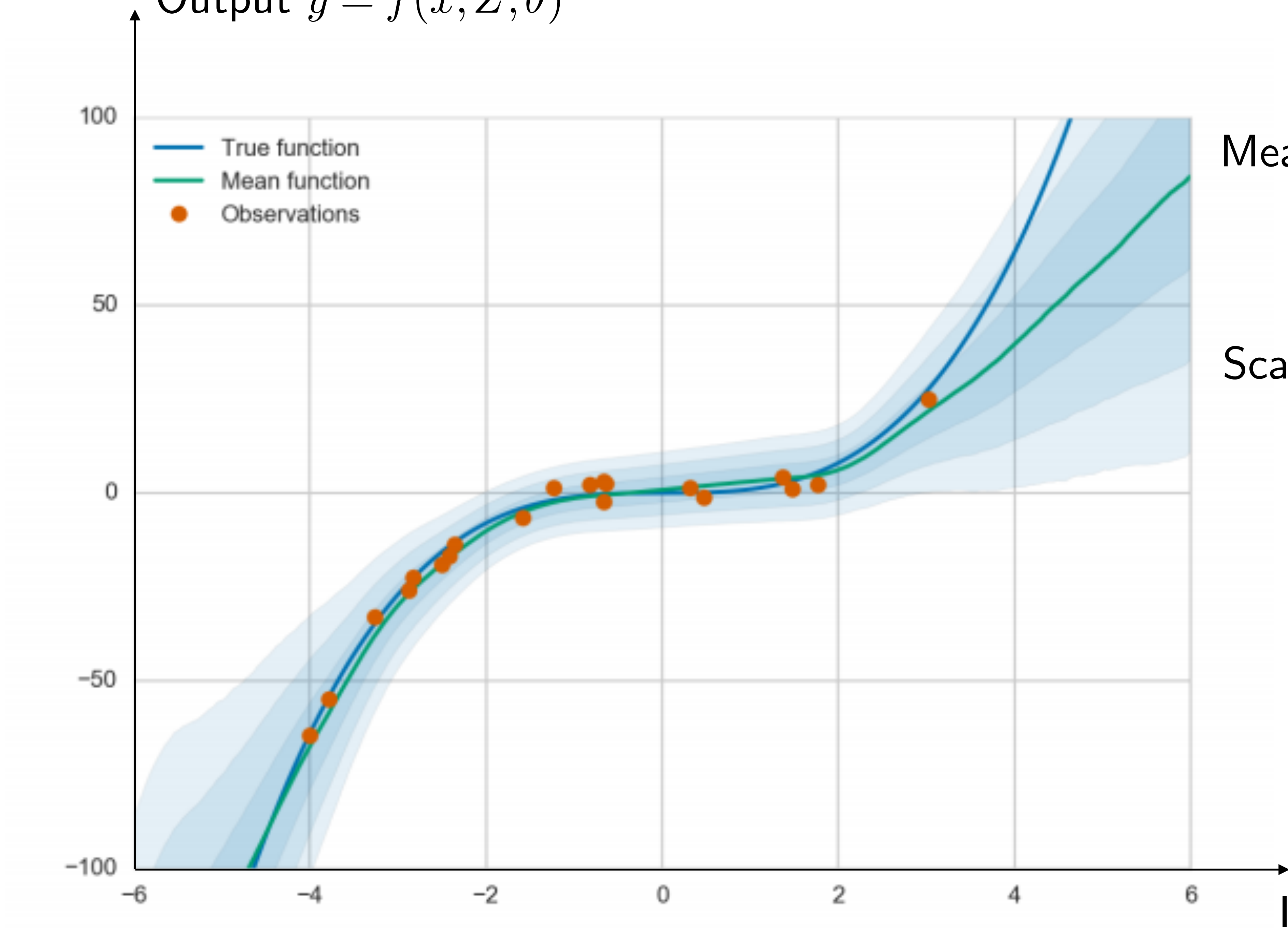


- More accurate analytic approximations than the first option are possible

Model Uncertainty with Dropout

[Louizos and Welling 2017]

Output $y = f(x, Z; \theta)$

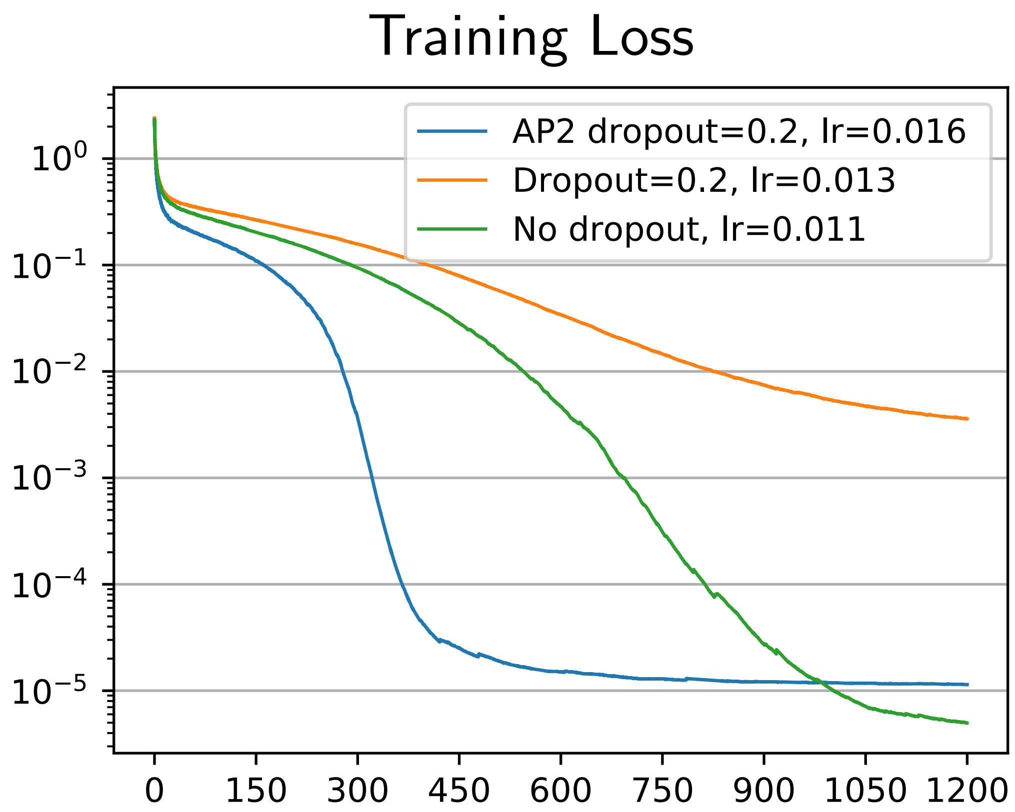


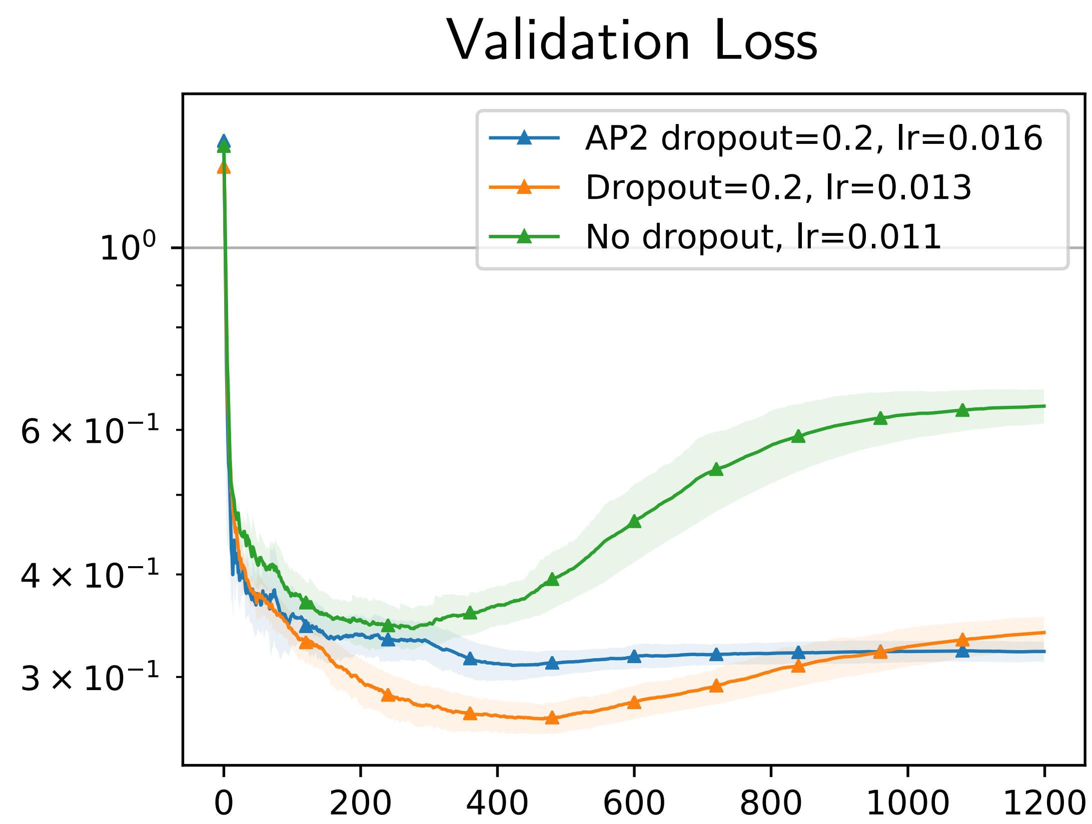
Input x

Mean of the ensemble

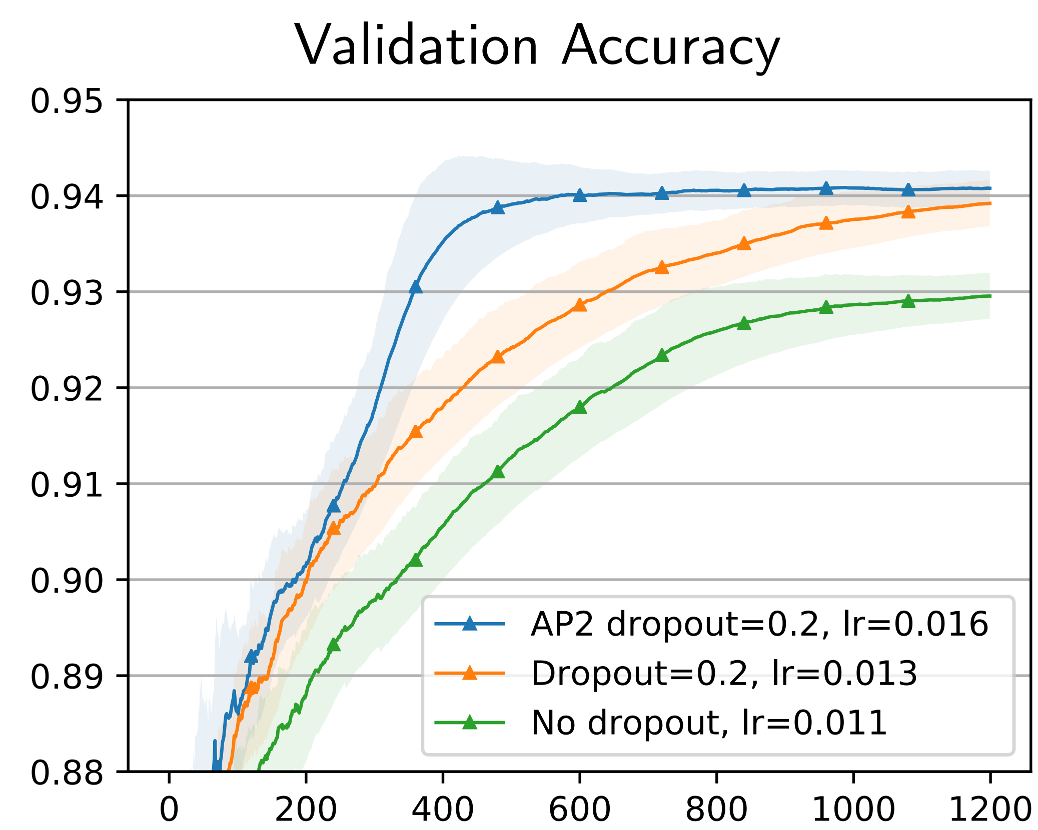
Scatter of the ensemble

CIFAR10 Example: Dropout





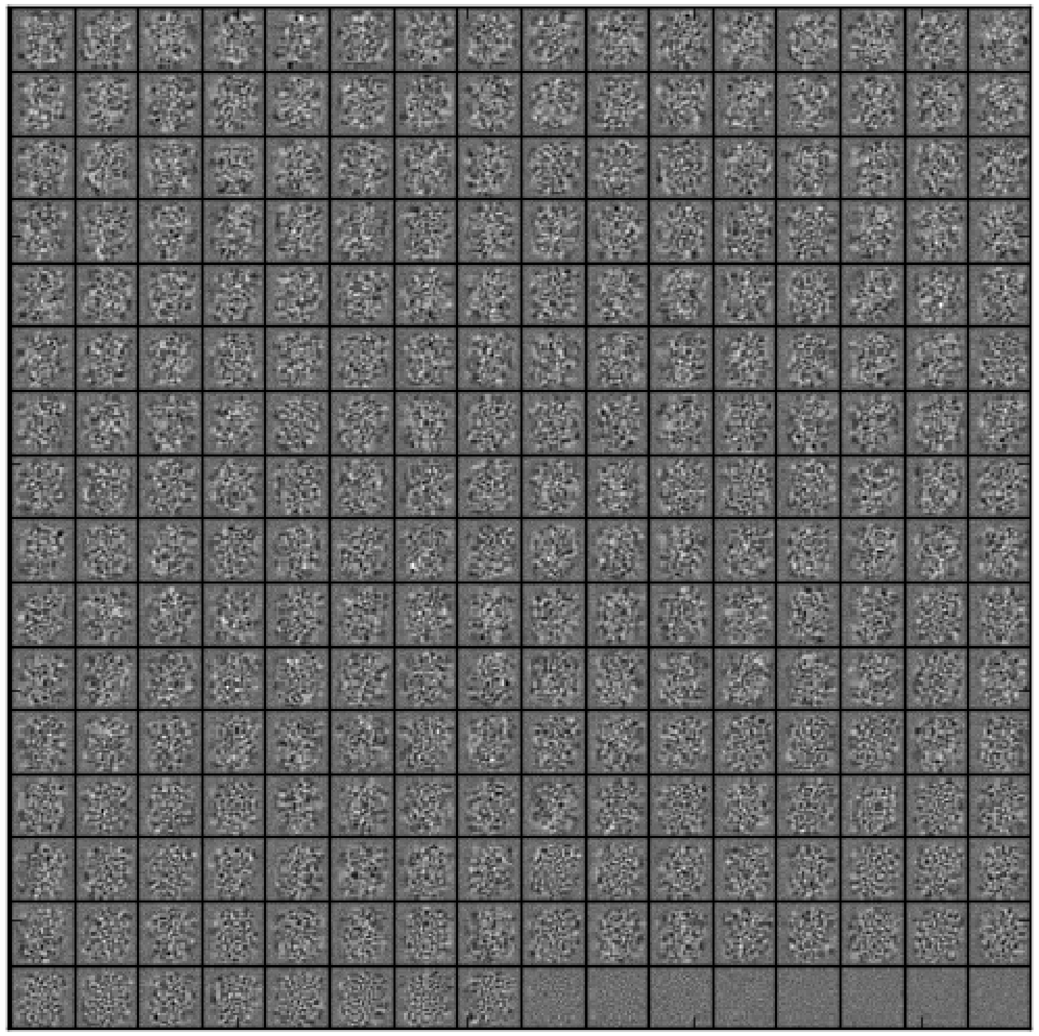
- Typically need to train longer due to higher gradient variance
  - There are techniques to approximate the effect analytically: Fast Dropout, Analytic Dropout (AP2)



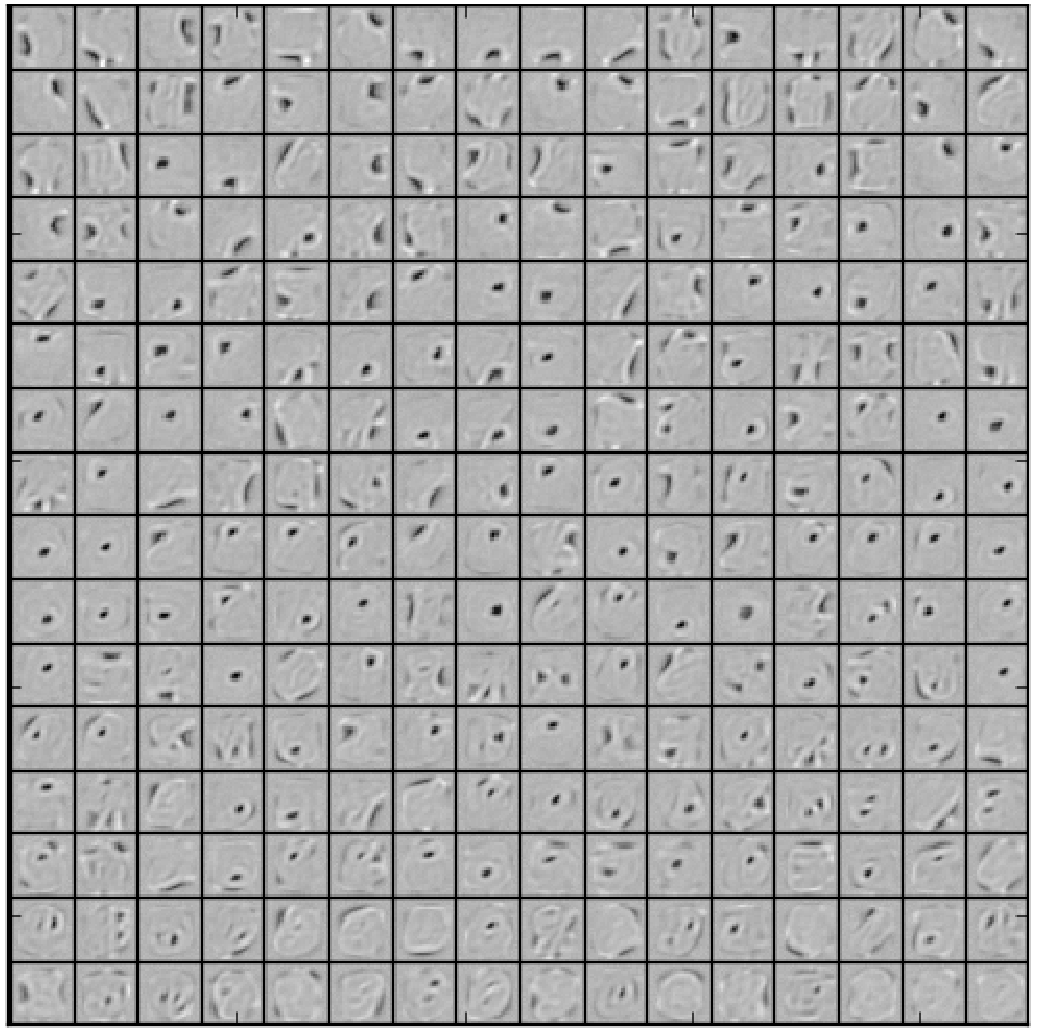
Effect on Features

✦ Experiment:

- MNIST auto encoder with 1 fully-connected hidden layer of 256 units



(a) Without dropout



(b) Dropout with $p = 0.5$.

[Srivastava et al. (2014)]

✦ Hypothehis: dropout prevents co-adaptation (learns simpler and more robust features)

✦ Further interesting studies in the paper: effect on activation sparsity, connection to ridge regression, etc.