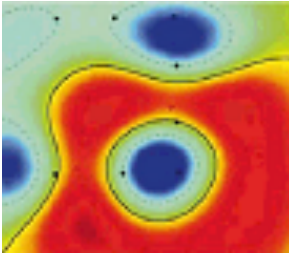


Lecture 9

Neural Networks 2

Outline

- Recap:
  - The Perceptron
  - Artificial Neural Networks
  - Forward / Backward Propagation
- Optimizing Neural Networks:
  - Bad Local Minima and Pathological Curvature
  - Initialization / Centering / Momentum
- Regularizing Neural Networks:
  - Hinge Loss
  - Perturbations

Recap: The Perceptron

F. Rosenblatt (1928–1971)

- Proposed by F. Rosenblatt in 1958.
- Classifier that perfectly separates training data (if the data is linearly separable).
- Trained using a simple and cheap iterative procedure.
- The perceptron gave rise to artificial neural networks.

Recap: The Perceptron Algorithm

Consider the linear model $y = \boldsymbol{w}^\top \boldsymbol{x} + b$, where $\text{sign}(y)$ gives the classification decision. Let $t \in \{-1, +1\}$ be the binary class label associated to $\boldsymbol{x}$.

Algorithm

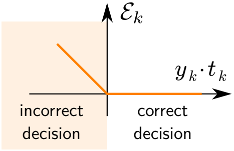
- Iterate over all data points $\{(\boldsymbol{x}_k, t_k)\,;\, k = 1 \dots, N\}$ (multiple times).
  - Compute $y_k = \boldsymbol{w}^\top \boldsymbol{x}_k + b$
  - If $\boldsymbol{x}_k$ is correctly classified (i.e. $\text{sign}(y_k) = t_k$), continue.
  - If $\boldsymbol{x}_k$ is wrongly classified (i.e. $\text{sign}(y_k) \neq t_k$), apply:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \gamma \cdot \boldsymbol{x}_k t_k \quad \text{and} \quad b \leftarrow b + \gamma \cdot t_k$$

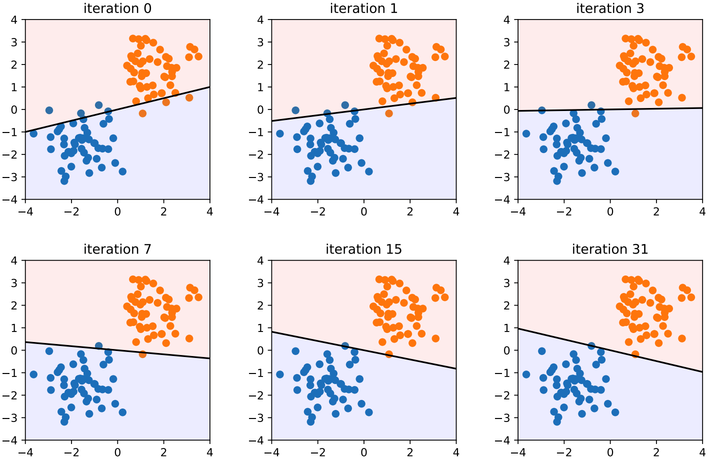
- Stop once all examples are correctly classified.

The perceptron can also be seen as a stochastic gradient descent of the error function

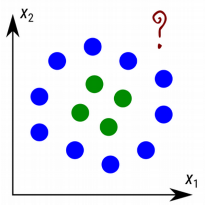
$$\mathcal{E}(\boldsymbol{w}, b) = \frac{1}{N} \sum_{k=1}^{N} \underbrace{\max(0, -y_k t_k)}_{\mathcal{E}_k(\boldsymbol{w}, b)}$$



Recap: Perceptron at Work



Recap: Nonlinear Classification



Observation:

- The perceptron builds a decision function which is linear in input space.
- In practice, the data may not be linearly separable.

Key Idea:

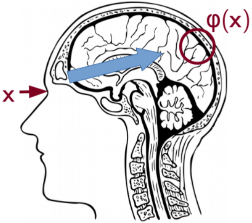
- Transform the data nonlinearly through some function Φ before applying the linear decision function.

$$f(\boldsymbol{x}) = \boldsymbol{w}^\top \Phi(\boldsymbol{x}) + b$$

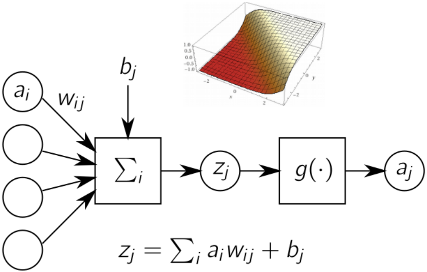
- *Example:* $\Phi(\boldsymbol{x}) = [x_1, x_2, x_1^2, x_2^2, x_1 x_2]$ and $\boldsymbol{w} \in \mathbb{R}^5$.

Recap: Artificial Neural Networks

- Models that are inspired by the way the brain represents sensory input and learn from repeated stimuli.
- Neuron activations can be seen as a nonlinear transformation of the sensory input (similar to $\Phi(\boldsymbol{x})$).
- The neural representation adapts itself after repeated exposure to certain stimuli (plasticity).



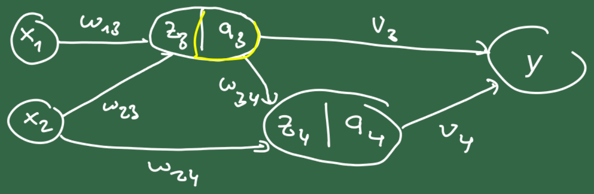
Recap: The Artificial Neuron



$$z_j = \sum_i a_i w_{ij} + b_j$$
$$a_j = g(z_j)$$

- Simple multivariate, nonlinear and differentiable function.
- Ultra-simplification of the biological neuron that retains two key properties: (1) ability to produce complex nonlinear representations when many neurons are interconnected (2) ability to learn from the data.

Recap: Artificial Neural Networks



$$z_3 = x_1 w_{13} + x_2 w_{23} \qquad a_3 = g(z_3)$$

$$z_4 = x_2 w_{24} + a_3 w_{34} \qquad a_4 = g(z_4)$$

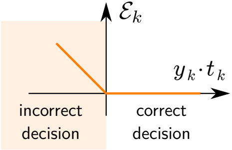
$$y = a_3 \cdot v_3 + a_4 v_4$$

Recap: Training a Neural Network

Idea:

- Use the same error function as the perceptron, but replace the perceptron output by the neural network output:

$$\mathcal{E}(\theta) = \frac{1}{N}\sum_{k=1}^{N} \underbrace{\max(0, -y_k t_k)}_{\mathcal{E}_k(\theta)}$$



and compute the gradient of the error function w.r.t. the parameters θ of the neural network.

Question:

- How to compute the gradient of the error function?

Recap: Error Backpropagation

Idea:

- The gradient can be expressed in terms of gradient in the higher layers using the multivariate chain rule.

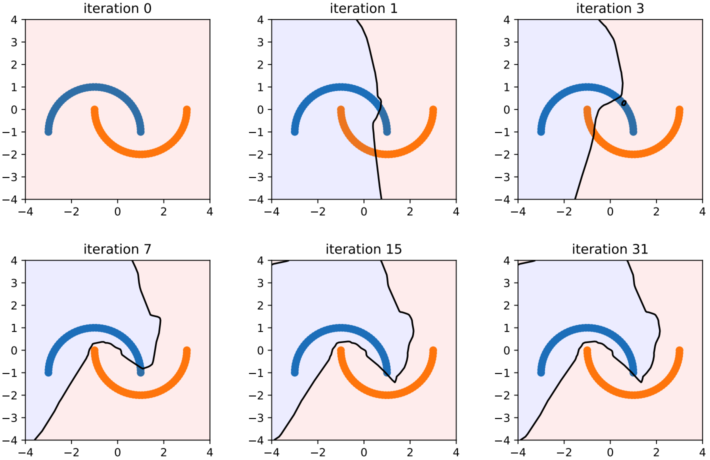
$$\frac{\partial \mathcal{E}}{\partial z_i} = \sum_j \frac{\partial z_j}{\partial z_i} \frac{\partial \mathcal{E}}{\partial z_j}$$

- Similarly, one can then extract the gradient w.r.t. the parameters of the model as:

$$\frac{\partial \mathcal{E}}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}} \frac{\partial \mathcal{E}}{\partial z_j}$$

- Gradients can be computed one after the other in a message passing fashion in O(forward pass). The algorithm is known as *error backpropagation*.

Recap: Neural Network at Work



Today's Lecture

Part 1:

- Optimizing Neural Networks
  (making sure neural networks can be trained effectively and efficiently).

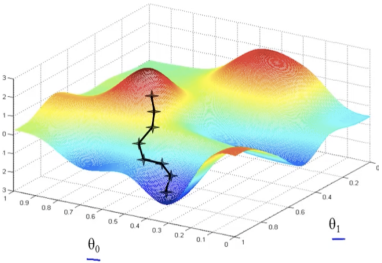
Part 2:

- Regularizing Neural Networks
  (making sure the learned models are good and generalize well).

Part 1: Optimizing Neural Networks

Questions:

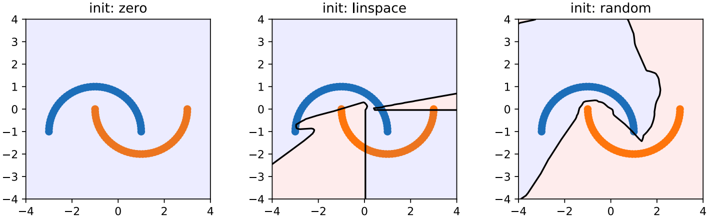
- How hard is it to optimize a neural network?
- Are we guaranteed to converge to a good local minimum?
- How quickly do we converge to this local minimum?



Neural Networks: Initialization

Experiment:

- Train the network with different weight initializations:



Observations:

- Some runs do not converge to a solution that perfectly classifies the data (e.g. when weights are initialized to zero, training is stuck on a plateau corresponding to a constant classifier).

某些训练运行无法收敛到一个能够完美分类数据的解决方案（例如，当权重初始化为零时，训练会卡在对应于常数分类器的平坦区域上）。

Neural Networks: Initialization

权重应随机初始化（这样可以打破参数空间中的对称性，并减少落入糟糕的局部极小值或陷入平坦区域的风险）。

如果有必要，可以用不同的随机种子多次训练网络，并保留误差最小的网络。

- Weights should be initialized *randomly* (it breaks symmetries in parameter space and reduces the risk of landing in bad local minima or getting stuck on plateaus).
- If necessary, train the network *multiple times* using different random seeds, and retain the network with the *lowest error*.

He-et-al[1] random initialization heuristic:

For neural networks with ReLU neurons, it is recommended to use: $w_{ij} \sim \mathcal{N}(0, \sigma^2)$ with $\sigma = \sqrt{2/\#\text{ input connections}}$ and where $\mathcal{N}$ is the Gaussian distribution.

Example: For a two-layer neural network with 50 *input features,* 200 *hidden neurons, and* 1 *output, weights in the first layer should be initialized using* $\sigma = \sqrt{2/50}$*, and in the second layer using* $\sigma = \sqrt{2/200}$.

[1] He et al. (2015) Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification

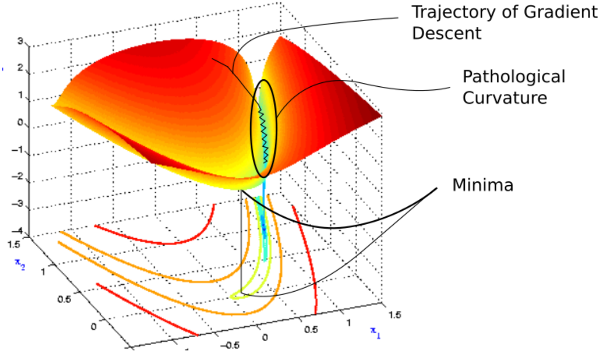
Neural Networks: Pathological Curvature

神经网络：病态曲率

另一个问题：

由于误差函数的**病态曲率**，神经网络可能会收敛到某个较好的局部最优解，但收敛速度非常缓慢。

Another problem: The neural network may converge to some good local optimum but slowly due to *pathological curvature* of the error function.



Source: Martens. Deep Learning via Hessian-free Optimization U Toronto, 2010.

Neural Networks: Pathological Curvature

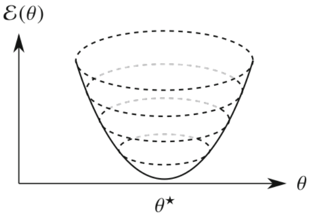
可以通过观察误差函数的海森矩阵（Hessian Matrix）的特征值来描述误差函数的曲率：

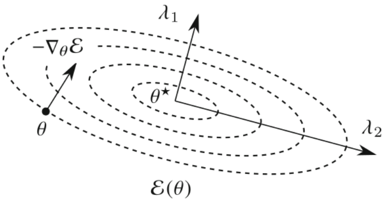
The curvature of the error function can be characterized by looking at the eigenvalues of the Hessian of the error function:

$$H = \left(\frac{\partial^2 \mathcal{E}(\theta)}{\partial\theta_i \partial\theta_j}\right)_{ij} \qquad \lambda_1, \dots, \lambda_{|\theta|} = \mathrm{eigvals}(H)$$

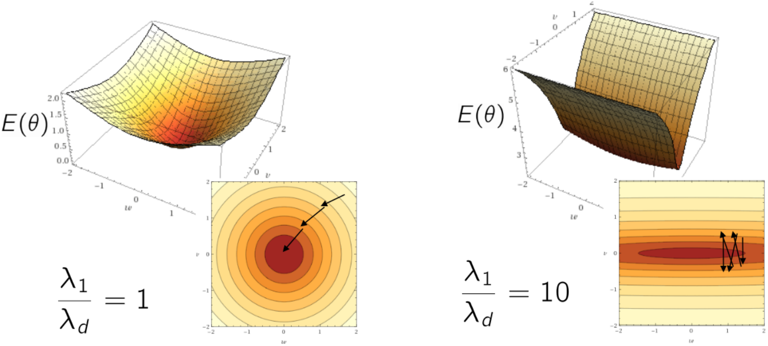
The higher the ratio between the highest and the lowest eigenvalue (aka. condition number), the slower the convergence.

Two-dimensional example:





Neural Networks: Pathological Curvature

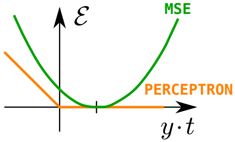


The lower the condition number, the better.

lamda_1 is the largest eigenvalue

Hessian Analysis (Linear Case, MSE)

Consider the simplest case of a homogeneous linear model $y = \boldsymbol{w}^\top \boldsymbol{x}$. Consider $\mathcal{E}(\boldsymbol{w}) = \mathbb{E}[0.5 \cdot (1 - y \cdot t)^2]$, the mean square error (MSE), which is easier to analyze than the perceptron loss.



The Hessian of the error function is given by:

$$H = \frac{\partial^2 \mathcal{E}}{\partial \boldsymbol{w}^2} = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^\top]$$

i.e. the data uncentered covariance.

Condition Number: Assuming $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \sigma^2 I)$,the Hessian reduces to $H = \sigma^2 I + \boldsymbol{\mu}\boldsymbol{\mu}^\top$, and the condition number is

$$\frac{\lambda_1}{\lambda_d} = 1 + \frac{\|\boldsymbol{\mu}\|^2}{\sigma^2}.$$

(show this in the homework). In other words, the condition number can be reduced by **centering the data** before training.

Hessian Analysis (General Case, MSE)

$\frac{\partial \mathcal{E}}{\partial Y}\left(\frac{\partial Y}{\partial \theta}^\top \frac{\partial \mathcal{E}}{\partial Y}\frac{\partial Y}{\partial \theta} + \frac{\partial^2 Y}{\partial \theta^2}\right)$

- Hessian of a neural network (LeCun et al. 1998):

$$H = \frac{\partial^2 \mathcal{E}}{\partial \theta^2} = \frac{\partial Y}{\partial \theta}^\top \frac{\partial^2 \mathcal{E}}{\partial Y^2} \frac{\partial Y}{\partial \theta} + \frac{\partial \mathcal{E}}{\partial Y} \frac{\partial^2 Y}{\partial \theta^2} \tag{1}$$

  where Y is the vector containing the predictions for all data points.

- Consider the part of the Hessian relating parameters of a specific neuron k. From Eq. (1), and assuming MSE, we get:

$$[H_k]_{jj'} = \frac{\partial^2 \mathcal{E}}{\partial w_{jk} \partial w_{j'k}} = \mathbb{E}[a_j a_{j'} \delta_k^2] + \mathbb{E}[a_j \frac{\partial \delta_k}{\partial w_{j'k}} \cdot (y - t)]$$

  where δ_k is a shortcut notation for $\partial \mathcal{E} / \partial z_k$.

- Assuming $a_j a_{j'}$ and δ_k^2 to be independent, and δ_k insensitive to $w_{j'k}$, we get:

$$H_k \approx \mathbb{E}[\boldsymbol{a}\boldsymbol{a}^\top] \cdot \mathbb{E}[\delta_k^2]$$

  which has a similar structure as in the analysis for the linear case.

- This motivates **centering activations** as well.

Hessian Analysis: Takeaway Message

为了降低条件数，并从而简化神经网络的优化过程：

使输入数据居中，并确保每一层的激活值也居中。

注意：

在实际中精确地使激活值居中可能很困难，但可以通过选择满足 $g(0) = 0$ 的激活函数来实现大致的居中。

To lower the condition number and consequently ease optimization of the neural network:

Center the input data, and also activations at each layer.

Note: Exactly centering activations can be difficult in practice, however, reasonably centered activations can be promoted by choosing an activation function satisfying $g(0) = 0$.

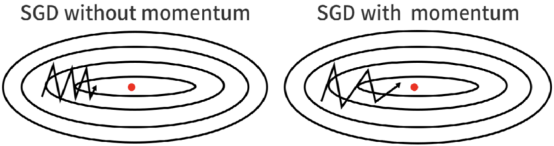
- Examples of **suitable** activation functions (where $g(0) = 0$) are the *ReLU* ($\max(0, z)$), the *centered softplus* ($\log(1 + \exp(z)) - \log(2)$), or the *hyperbolic tangent* ($\tanh(z)$).
- Examples of **less suitable** activation functions (where $g(0) \neq 0$) are the *standard softplus* ($\log(1 + \exp(z))$), or the *logistic sigmoid* ($\exp(z)/(1 + \exp(z))$).

Improving Gradient Descent

改进梯度下降

- **居中**可能显著减少误差函数的病态曲率，但不能完全消除它（尤其是对于深度神经网络而言）。
- **一种补充方法：**可以通过修改优化方法，使其沿低曲率方向加速移动。
- 这可以通过在梯度下降中引入**动量（momentum）**来实现。

- Centering may significantly reduce the pathological curvature, but does not completely eliminate it (especially for deep neural networks).
- A complementary approach to centering is to modify the optimization procedure to move faster along directions of low curvature.
- This can be achieved by introducing a '*momentum*' in the gradient descent:



Improving Gradient Descent

(Stochastic) Gradient Descent:

$$\theta = \theta - \gamma \cdot \frac{\partial \mathcal{E}_k}{\partial \theta} \qquad \text{with} \quad k \sim \{1, \dots, N\}$$

where γ is the learning rate.

(Stochastic) Gradient Descent + Momentum:

$$\Delta_{\text{new}} = \mu \Delta_{\text{old}} + \frac{\partial \mathcal{E}_k}{\partial \theta} \qquad \text{with} \quad k \sim \{1, \dots, N\}$$

$$\theta = \theta - \gamma \Delta_{\text{new}}$$

where γ is the learning rate and μ is the momentum.

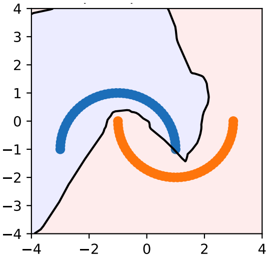
Heuristics:

- Typical learning rate and momentum: $\gamma = 0.01$ and $\mu = 0.9$ (need to be reduced if training diverges).

Part 2: Regularizing Neural Networks

Questions:

- Do neural networks trained with gradient descent and the perceptron loss yield good models?
- How to help neural networks to learn solutions that generalize well to new data?



Learning Well-Generalizing Solutions

So far:

- We have used the perceptron loss:

$$\mathcal{E}_k(\theta) = \max(0, -y_k t_k)$$

which becomes zero as soon as the current data point is being correctly classified.

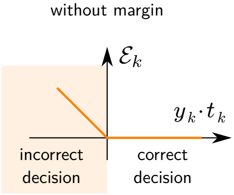
Idea: 对离决策边界过近的点（即添加一个间隔）施加惩罚，也就是 **Hinge 损失**（Hinge Loss）：

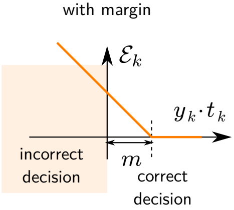
- Impose a penalty to points that lie too close to the decision boundary (i.e. add a margin), aka. the Hinge Loss:

$$\mathcal{E}_k(\theta) = \max(0, 1 - y_k t_k)$$

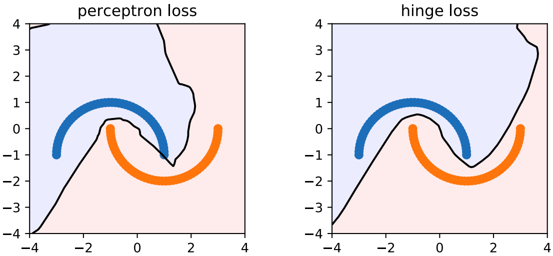
This is similar to the slack variables penalties in the soft-margin SVM formulation.

这类似于软间隔支持向量机（SVM）公式中的松弛变量惩罚项。





Hinge Loss at Work



Observation:

- Using the hinge loss, the decision function of the neural network moves away from the data.
- This leads to a better generalization performance.

More Loss Functions

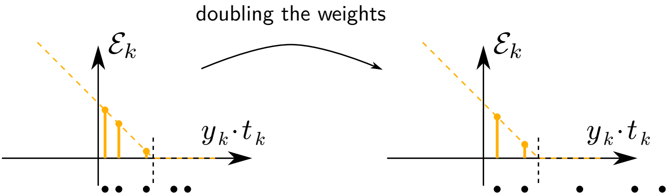
Name	Formula	Margin	Outliers[2]
Perceptron loss	$\max(0, -y \cdot t)$	no	yes
Hinge loss	$\max(0, 1 - y \cdot t)$	yes	yes
Squared hinge loss	$\max(0, 1 - y \cdot t)^2$	yes	no
Log-loss	$\log(1 + \exp(-y \cdot t))$	yes	yes

[2] Indicates whether the loss function is robust to outliers (e.g. mislabelings).

What is Still Missing?

Problem:

- If multiplying the weights by some factor, the hinge loss can be trivially reduced until it reaches zero, without actually changing the decision boundary.



- In the SVM, this was avoided by constraining $\|\boldsymbol{w}\|^2$ to be small.

Idea:

- To arrive at a well-generaling model, we also need to regularize the neural network itself.

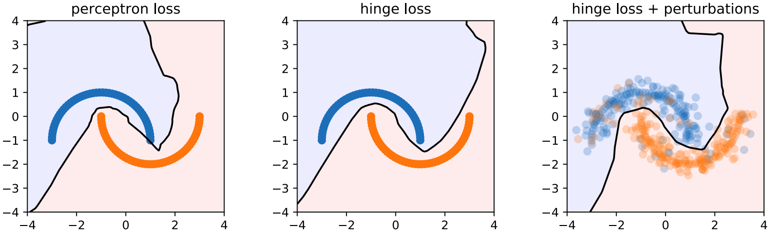
Regularizing the Neural N

- 权重衰减（Weight Decay）：
  在目标函数中添加一项 $\lambda \cdot ||\theta||^2$。
  这相当于在每次训练迭代中通过某个常数因子来缩小权重。
- 数据扰动（Data Perturbation）：
  对输入样本（例如，添加高斯噪声）和标签（随机翻转）应用随机扰动。
- 表示扰动（Representation Perturbation）：
  Dropout 方法（Srivastava，2014）将数据扰动的概念扩展到中间表示层，训练时随机关闭和开启神经元。
- 训练噪声（Training Noise）：
  已发现随机梯度下降（SGD）与标准梯度下降相比具有正则化效果。

Many approaches have been proposed and are often combined in practice. Some of the most popular ones are:

- **Weight decay:** Add a term $\lambda \cdot ||\theta||^2$ to the objective. This is equivalent to multiplying the weights at each training iteration by some constant factor.
- **Data perturbation:** Apply random perturbations to the input examples (e.g. Gaussian additive noise), and to the labels (random flips).
- **Representation perturbation:** The Dropout method (Srivastava'14) extends the idea of data perturbation to intermediate representations, by randomly turning on and off neurons while training.
- **Training noise:** Stochastic gradient descent was found to have a regularizing effect compared to standard gradient descent.

Data Perturbation at Work



Observation:

- Data perturbations pull the decision boundary further away from the class manifolds, and typically further improves generalization.

数据扰动将决策边界进一步拉离类别流形（class manifolds），并通常进一步提高模型的泛化能力。

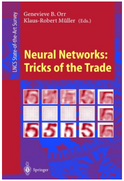
Neural Networks vs. SVMs/Kernels

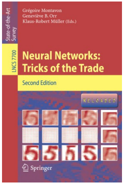
SVMs/Kernels:

- Relatively straightforward to optimize and regularize.
- Doesn't scale well to very large datasets with millions of examples.

Neural Networks:

- Can be trained on very large distributions (with GPUs).
- Challenging to optimize and regularize neural networks. Lots of tricks and heursistics involved. Can make results harder to reproduce and less transparent.



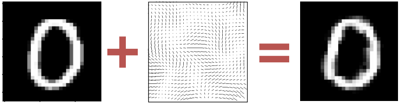
, 

, etc.

Neural Networks: Futher Topics

Further Topics:

- **Incorporate prior knowledge:** Data extension, weight sharing, unsupervised pretraining, self-supervised pretraining, transfer learning, multitask learning.



- **Predicting structured data:** Convolutional neural networks, recurrent neural networks, transformers, graph neural networks ($\rightarrow$ ML2).
- **Beyond classification:** Neural networks for regression, mixture density networks, structured prediction ($\rightarrow$ ML2).

对抗性鲁棒性 **Adversarial robustness:** Adversarial training, model certification.

- **Explainability:** Extracting insights from a neural network, Clever Hans effect (later this semester).

Summary

在实际应用中，神经网络面临两个主要挑战：

- **如何优化**它们
- **如何正则化**它们以便获得良好的泛化能力。

优化问题可以通过计算误差函数的海森矩阵（Hessian）和条件数（Condition number）来进行分析研究。

引入边际损失（Margin losses）和扰动（Perturbations）可以获得良好泛化能力的模型。

Previous lecture:

- Neural networks derive their **high representation power** from a large number of simple interconnected components (neurons), and the gradient of a neural network w.r.t. its parameters can be efficiently extracted (using **backpropagation**).

Today's lecture:

- In practice, there are two major challenges with neural networks (1) how to **optimize** them, and (2) how to **regularize** them so that they generalize well.
- The problem of optimization can be studied analytically by computing the **Hessian** of the error function and the **condition number**.
- Well-generalizing models can be obtained by introducing **margin losses** and **perturbations**.