Visual Computing Institute
RWTH AACHEN UNIVERSITY

Elements of Machine Learning & Data Science

Winter semester 2023/24

Lecture 19 – Neural Networks Basics

19.12.2023

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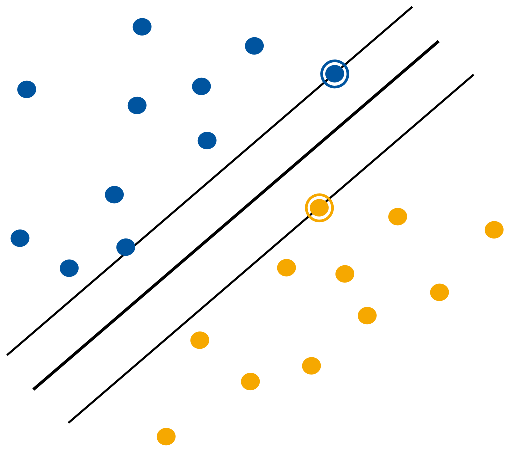
Machine Learning Topics

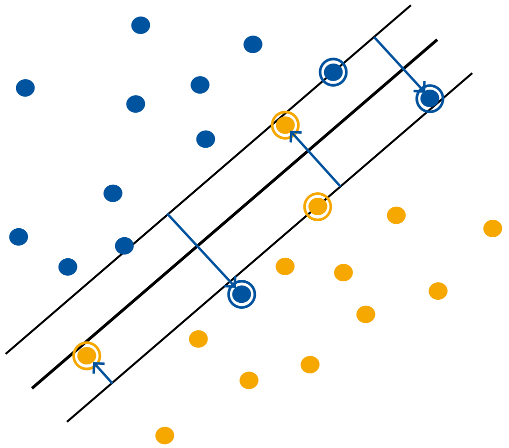
1. Introduction to ML
2. Probability Density Estimation
3. Linear Discriminants
4. Linear Regression
5. Logistic Regression
6. **Support Vector Machines**
7. (AdaBoost)
8. Neural Network Basics



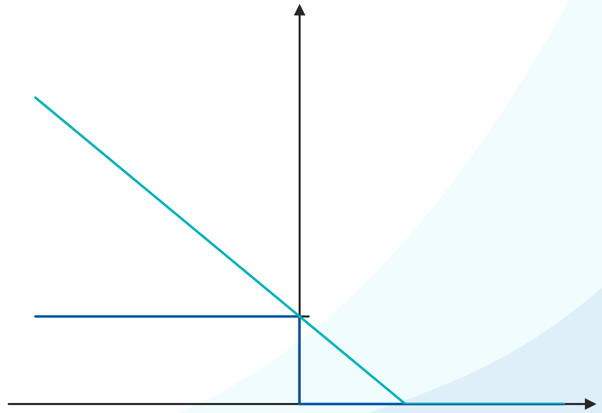
Maximum Margin Classification

$$L_p(\mathbf{w}, b, \mathbf{a})$$
$$L_d(\mathbf{a})$$

Primal & Dual Form



Soft-Margin SVM



Hinge Loss

Recap: Soft-Margin SVM

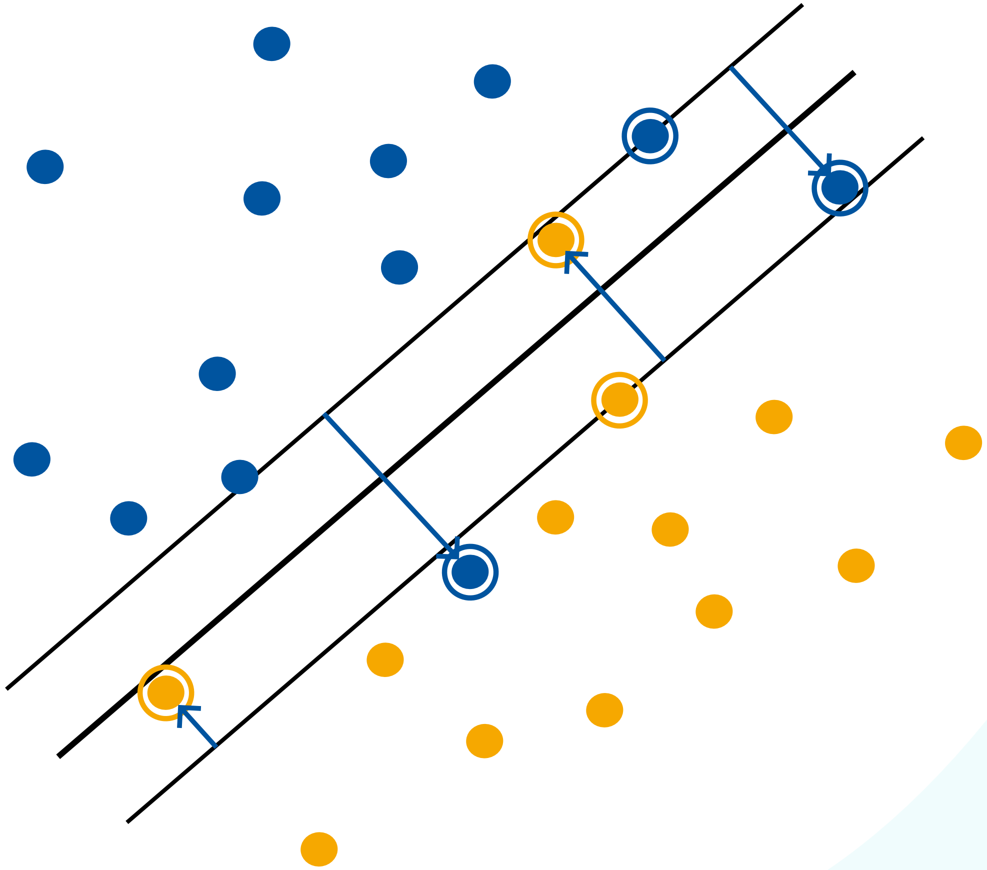
- Idea: Introduce slack variables $\xi_n \geq 0$
  - One slack variable ξ_n for each training point

- Effect
  - $\xi_n = 0$ for points on the correct side.
  - Linear penalty for all other points:
    $\xi_n = |t_n - y(\mathbf{x}_n)|$

- Slack variables are jointly optimized with $\mathbf{w}$:

$$\min \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

where C is a tradeoff parameter.



Recap: Soft-Margin SVM Primal Form

- Minimize

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \underbrace{\sum_{n=1}^{N} a_n \left[t_n(y(\mathbf{x}_n) - 1 + \xi_n\right]}_{\text{Constraint}} - \underbrace{\sum_{n=1}^{N}\mu_n\xi_n}_{\text{Constraint}}$$

Constraint $t_n y(\mathbf{x}_n) \geq 1 - \xi_n$

Constraint $\xi_n \geq 0$

- KKT conditions

$$\begin{aligned} a_n &\geq 0 & \mu_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 + \xi_n &\geq 0 & \xi_n &\geq 0 \\ a_n \left[t_n y(\mathbf{x}_n) - 1 + \xi_n\right] &= 0 & \mu_n\xi_n &= 0 \end{aligned}$$

Recap: Soft-Margin SVM Dual Form

- Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathsf{T}} \mathbf{x}_n)$$

- Under the side conditions

$$0 \leq a_n \leq C \quad \forall n$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

This is the only difference to before.

Recap: Non-linear SVM Formulation

- Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_m, \mathbf{x}_n)$$

under the constraints $\quad 0 \leq a_n \leq C \quad \forall n$

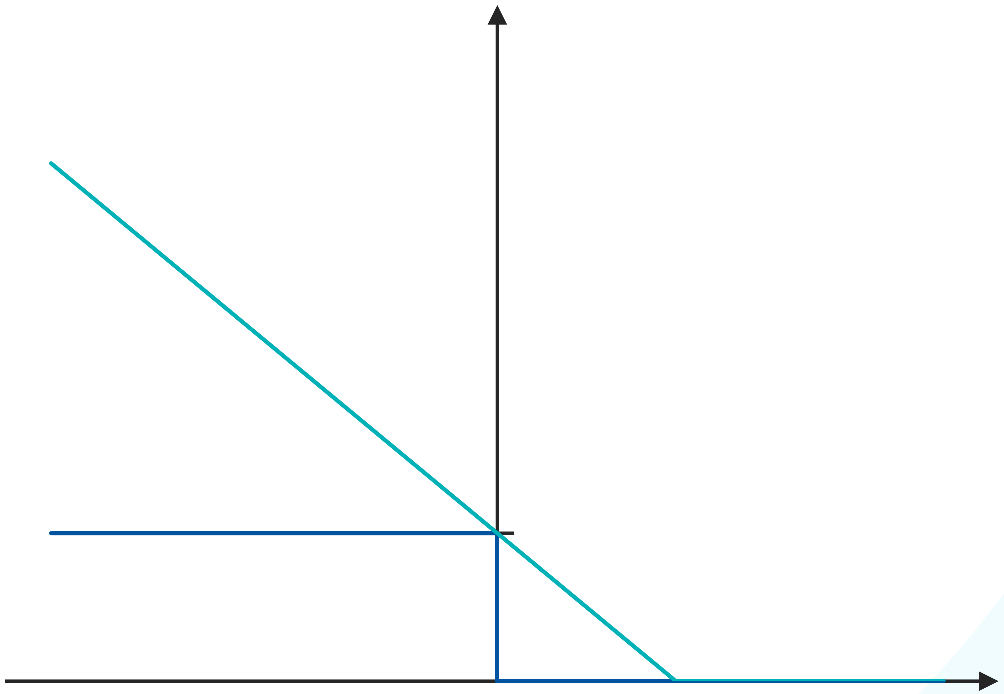
$$\sum_{n=1}^{N} a_n t_n = 0$$

- Classify new data points using

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

Support Vector Machines

1. Maximum Margin Classification
2. Primal Formulation
3. Dual Formulation
4. Soft-Margin SVMs
5. Non-linear SVMs
6. **Error Function Analysis**



Error Function Analysis

- We know how to formulate and optimize an SVM as a convex optimization problem:

$$\underset{\mathbf{w},\, b,\, \xi_n \in \mathbb{R}^+}{\arg\min} \; \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N} \xi_n$$

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n$$

Error Function Analysis

- We know how to formulate and optimize an SVM as a convex optimization problem:

$$\underset{\mathbf{w},\, b,\, \xi_n \in \mathbb{R}^+}{\arg\min} \; \frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{n=1}^{N} \xi_n$$

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n$$

But what error function does this correspond to?

- Integrate the constraints into the objective function:
  - Rewrite as $\xi_n \geq 1 - t_n y(\mathbf{x}_n)$
  - Thus, we obtain

$$\min_{\mathbf{w},\, b} E(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{n=1}^{N} [1 - t_n y(\mathbf{x}_n)]_+$$

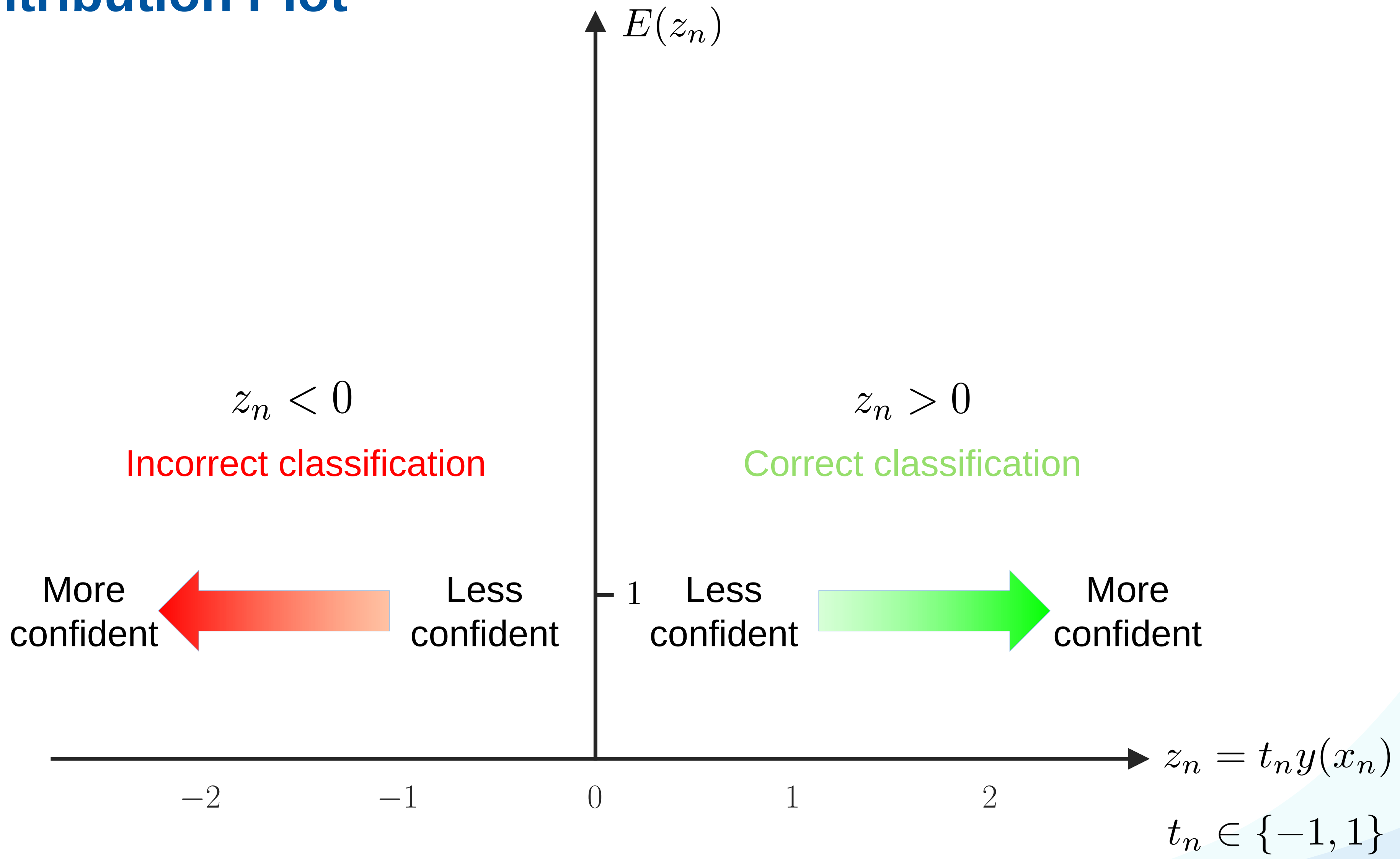
$$[x]_+ \equiv \max\{x, 0\}$$

The Hinge Loss

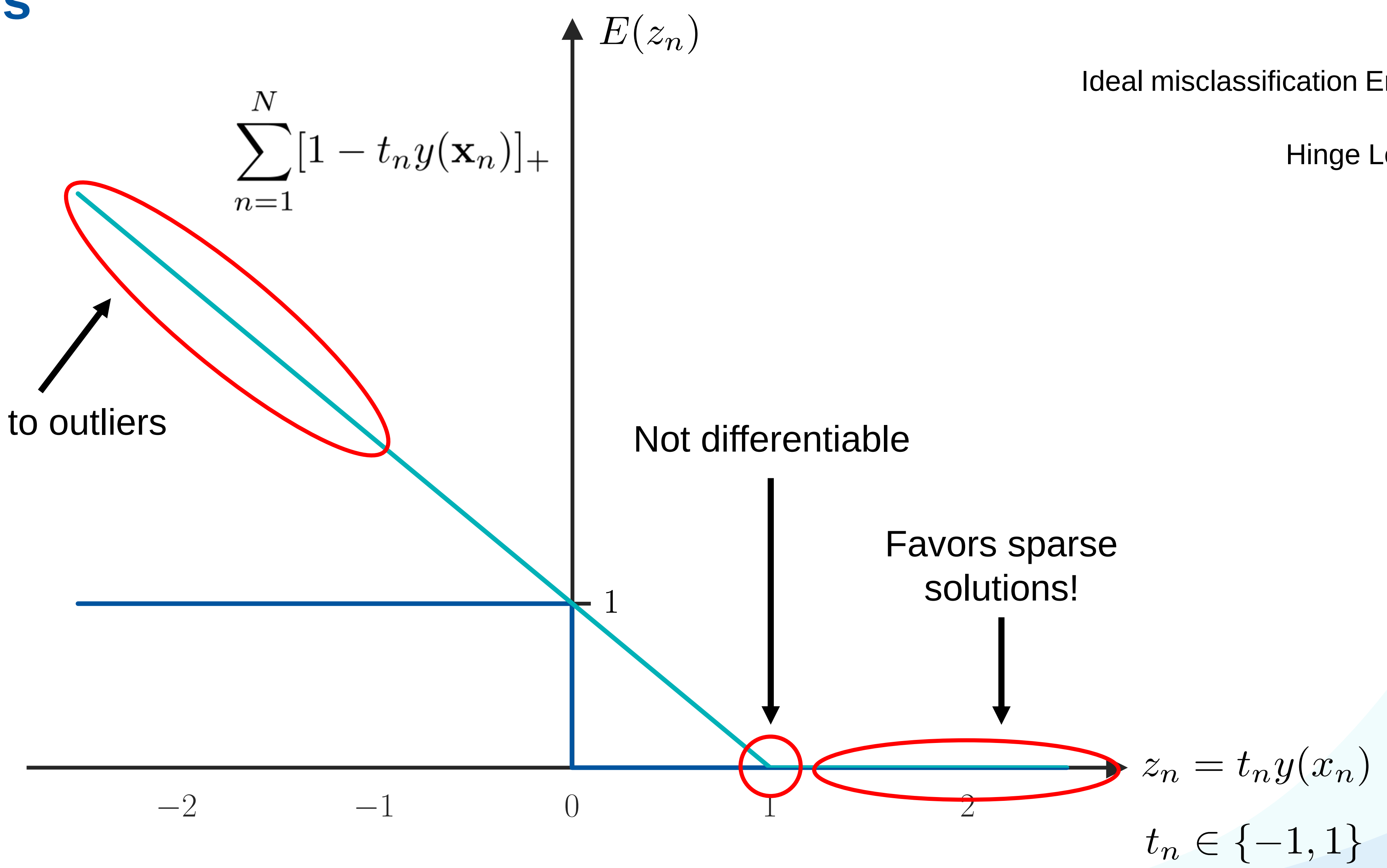
$$E(\mathbf{w}) = \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L}_2 \text{ regularization}} + \underbrace{C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{Hinge loss}}$$

- Regularization bounds parameter size.
- Hinge Loss enforces sparsity:
  - Only a subset of training data points actually influences the decision boundary.
  - Still, all input dimensions are used.
- This formulation corresponds to an unconstrained optimization of a non-differentiable function.
  - Very efficient: stochastic (sub-)gradient descent.

Error Contribution Plot

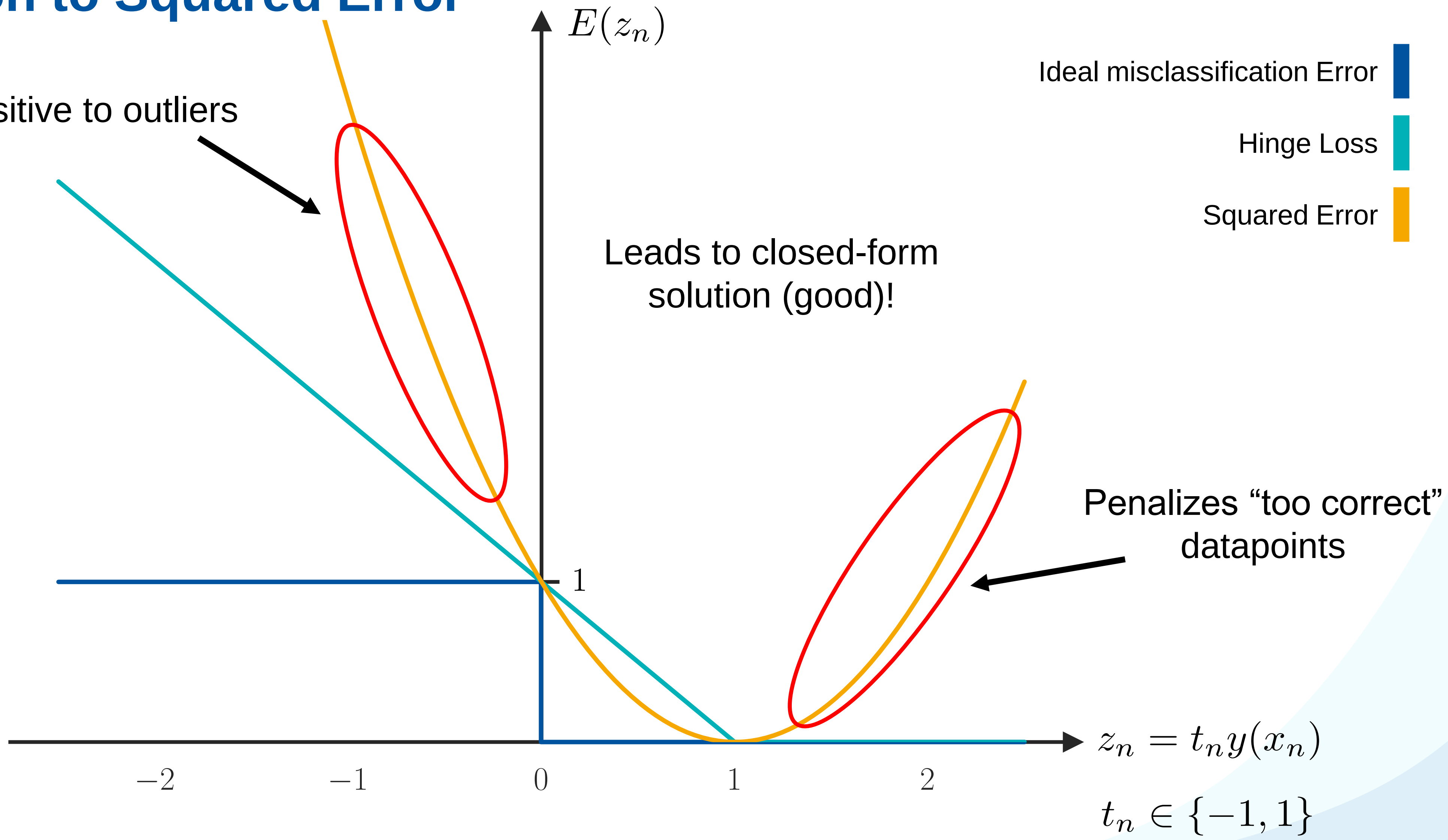


Hinge Loss

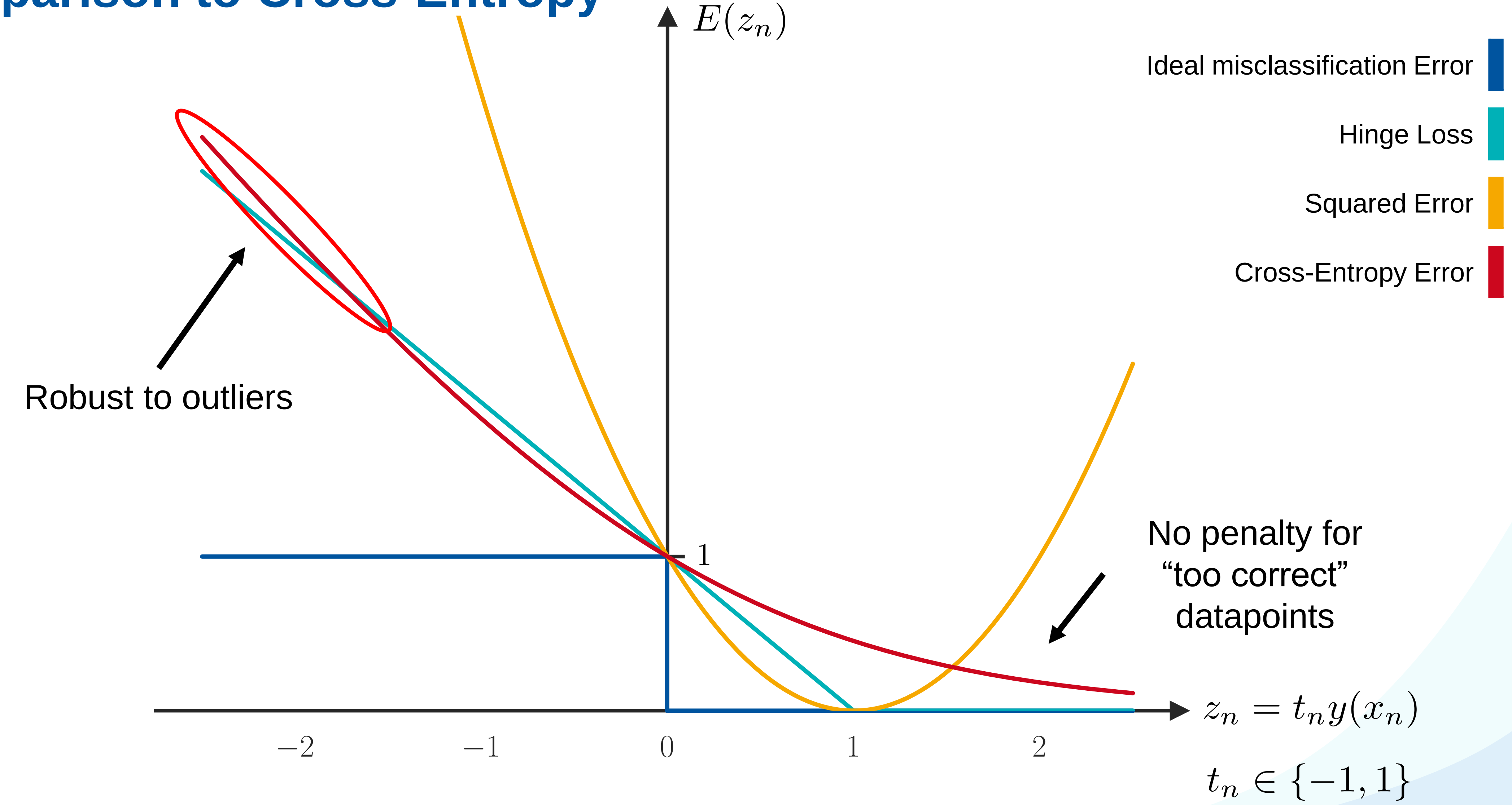


$E(z_n)$
Ideal misclassification Error
Hinge Loss
$\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+$
Robust to outliers
Not differentiable
Favors sparse solutions!
1
-2
-1
0
1
2
$z_n = t_n y(x_n)$
$t_n \in \{-1, 1\}$

Comparison to Squared Error



Comparison to Cross-Entropy



Discussion: Hinge Loss

Advantages

- Favors sparse solutions that only depend on a subset of training data points.
- Robust to outliers (only a linear penalty for misclassified points).
- Convex function, unique minimum exists.

Limitations

- Not differentiable (cannot minimize this loss using standard gradient descent, but need to use subgradient descent).

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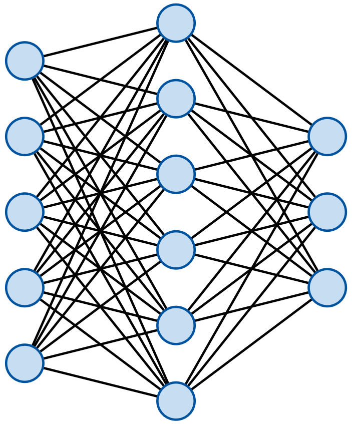
8. **Neural Network Basics**



Multi-Layer Perceptrons

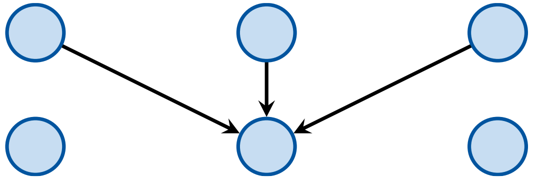
$$\frac{1}{2}(y(\mathbf{x})-t)^2$$

$$[1-ty(\mathbf{x})]_+$$

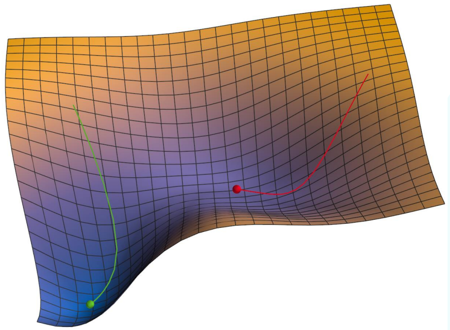
$$-\sum_k \left(\mathbb{I}(t=k)\ln \frac{\exp(y_k(\mathbf{x}))}{\sum_j \exp(y_j(\mathbf{x}))}\right)$$

$$\frac{1}{2}\|\mathbf{w}\|^2$$

Losses & Regularizers



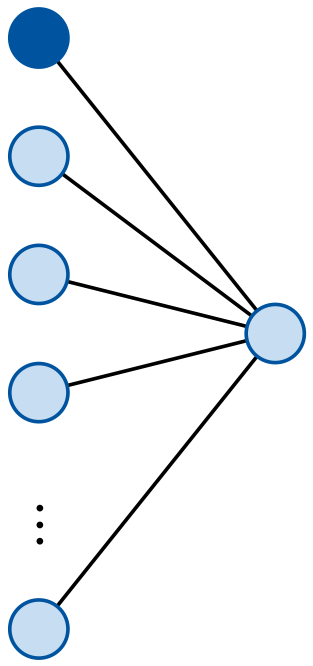
Backpropagation



Stochastic Gradient Descent

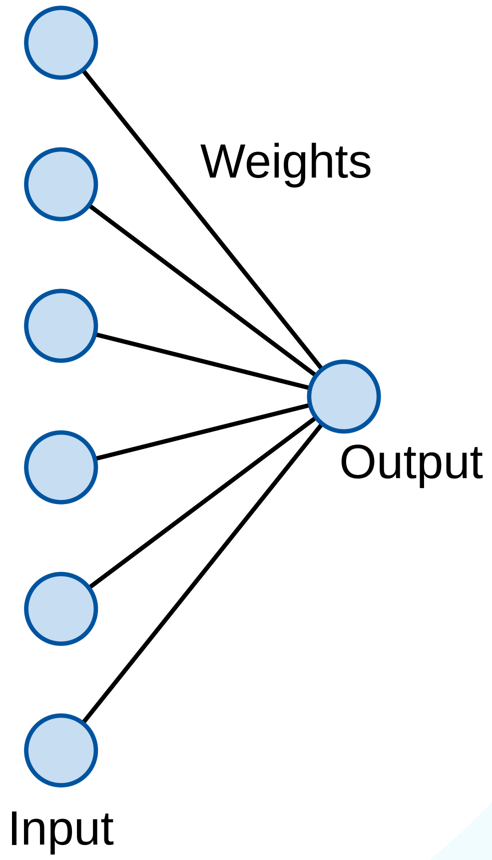
Neural Network Basics

1. **Perceptrons**
2. Multi-Layer Perceptrons
3. Loss Functions
4. Backpropagation
5. Stochastic Gradient Descent



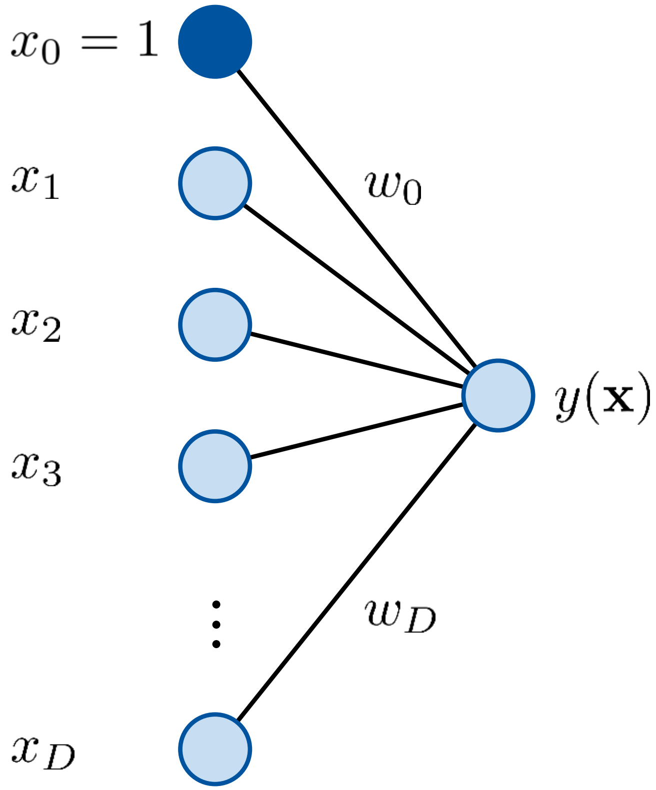
Perceptrons

- Inspired by biological neurons.
- The output is determined by the activation of the input nodes and a set of weights connecting input and output layers.



Basic Perceptron

- Input Layer:
  - Hand-designed features
- Outputs:
  - Linear outputs
    $$y(\mathbf{x}) = \mathbf{w}^\mathsf{T}\mathbf{x} + w_0$$
  - Logistic outputs
    $$y(\mathbf{x}) = \sigma(\mathbf{w}^\mathsf{T}\mathbf{x} + w_0)$$
- Learning: finding optimal weights $\mathbf{w}$.



Multi-Class Networks

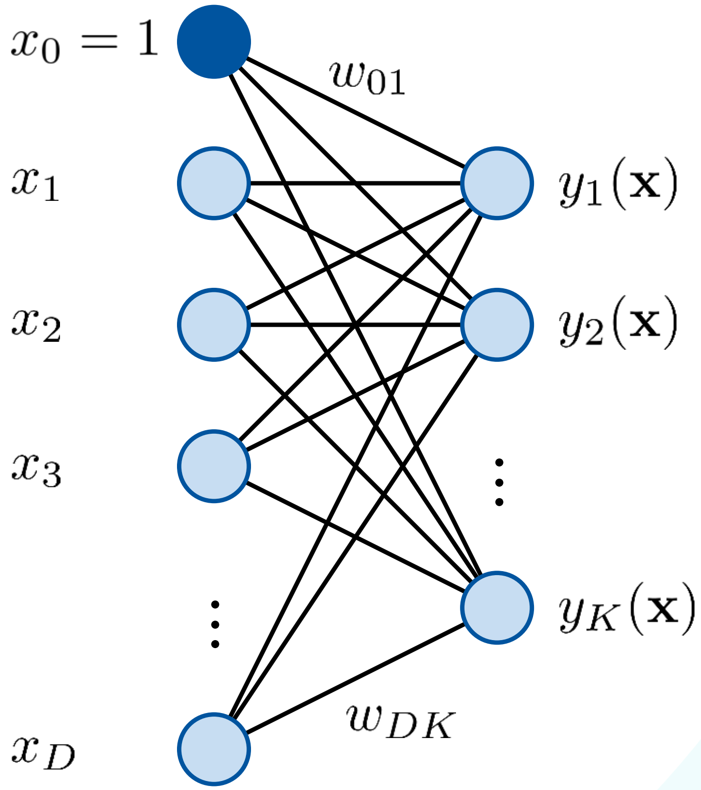
- One output node per class:
  - Linear outputs

$$y_k(\mathbf{x}) = \sum_{i=0}^{D} w_{ki}\mathbf{x}_i$$

  - Logistic outputs

$$y_k(\mathbf{x}) = \sigma\left(\sum_{i=0}^{D} w_{ki}\mathbf{x}_i\right)$$

- We can do multidimensional linear regression or multiclass classification this way.



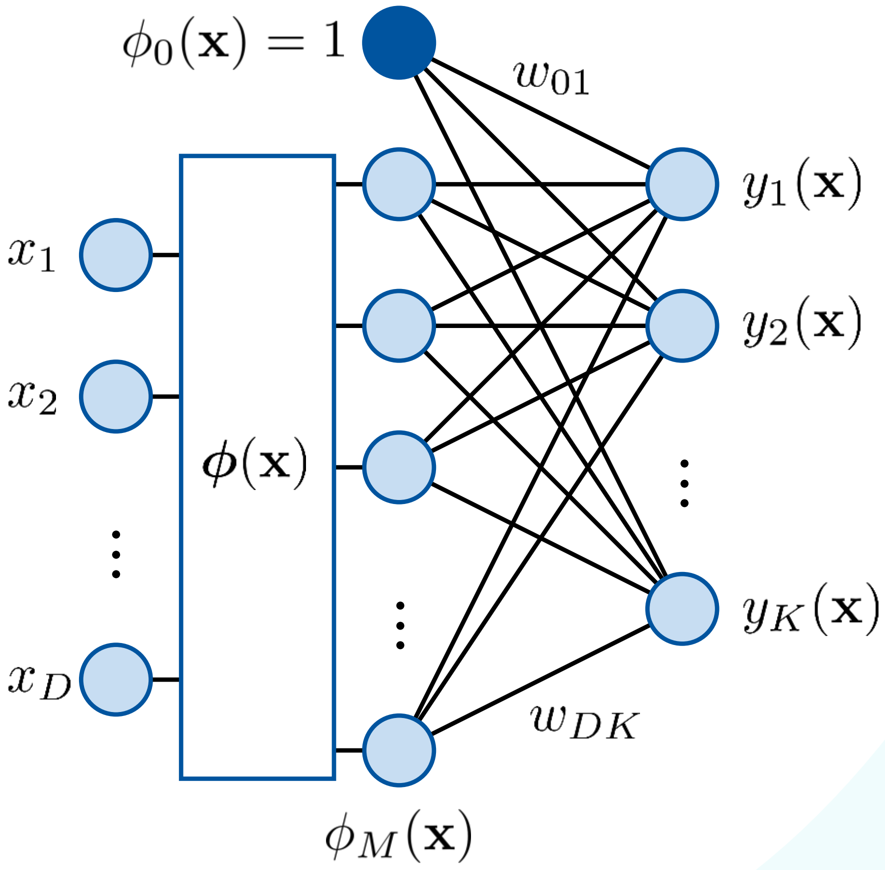
Non-Linear Basis Functions

- Apply a (fixed) mapping $\phi(\mathbf{x})$ to inputs:
  - Linear outputs

$$y_k(\mathbf{x}) = \sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})$$

  - Logistic outputs

$$y_k(\mathbf{x}) = \sigma\left(\sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x})\right)$$



Connections to linear discriminants

- All of this should feel very familiar.
- Perceptrons are generalized linear discriminants!

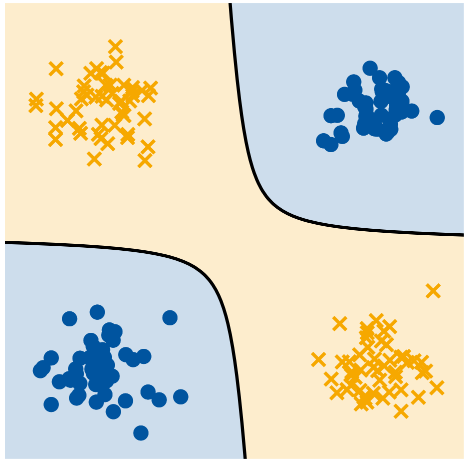
- What does that mean?
  - We have the same limitations as before.
  - Can model any separable function perfectly, given the right input features.
  - For some tasks, this may require an exponential number of input features.

$\Rightarrow$ *It is the feature design that solves the task!*

Limitations so far

- Generalized linear discriminants (including perceptrons) are very limited.
  - A linear classifier cannot solve certain problems (e.g., XOR).
  - However, with a non-linear classifier based on suitable features, the problem becomes solvable.
  - So far, we have designed the features and kernels by hand.

$\Rightarrow$ *How can we learn good feature representations?*



Neural Network Basics

1. Perceptrons
2. **Multi-Layer Perceptrons**
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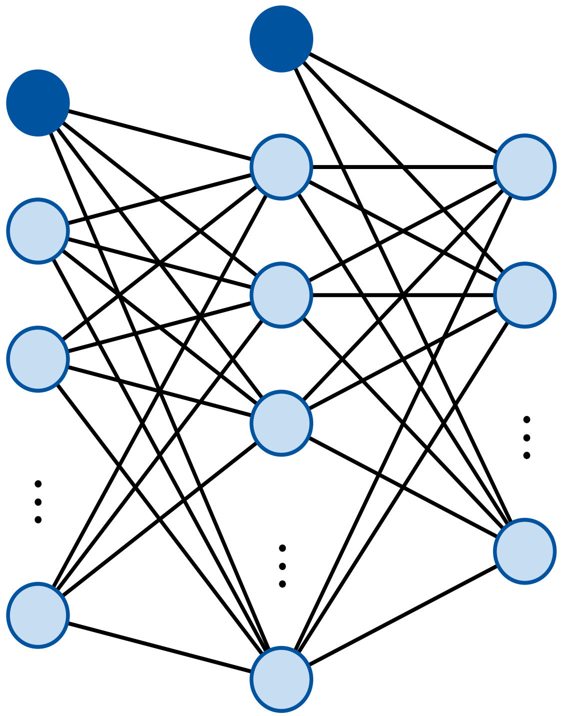
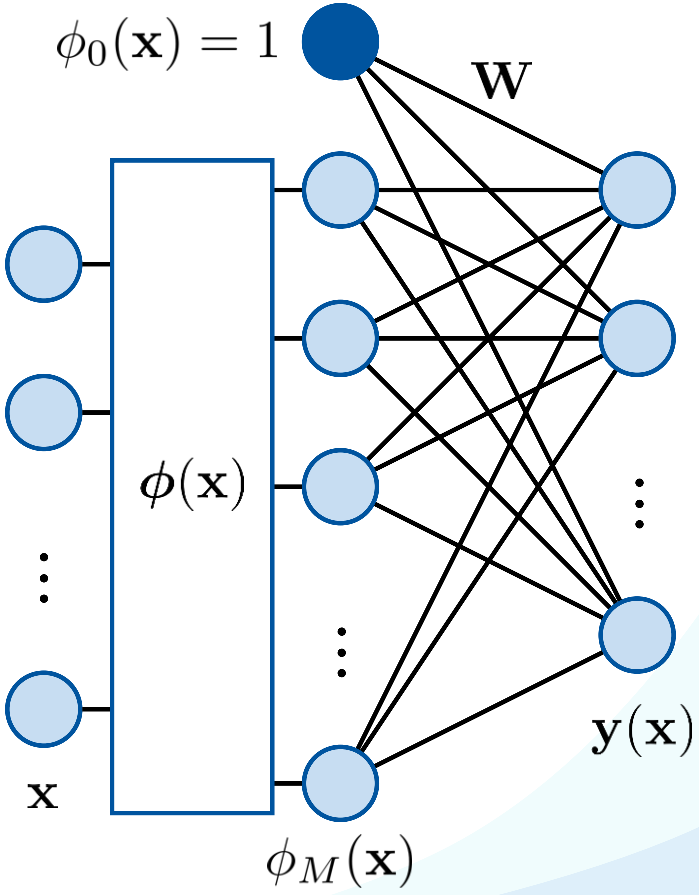


Multi-Layer Perceptrons

- Perceptrons are limited by having a fixed input mapping.

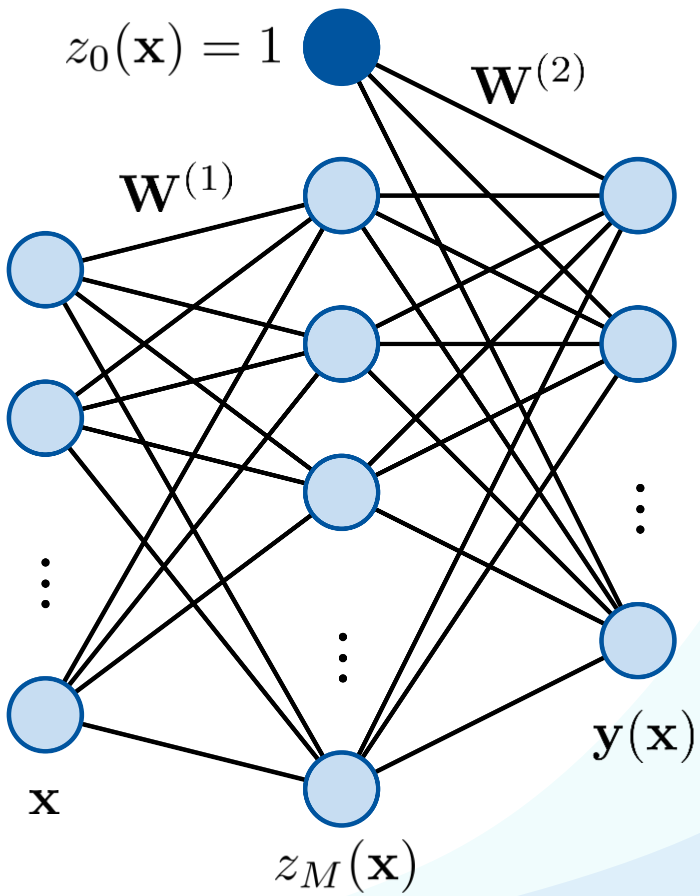


Multi-Layer Perceptrons

- Perceptrons are limited by having a fixed input mapping.
- Replace it with a hidden layer that learns suitable features.
- Output of hidden layer is input to next layer.
- Each layer computes a matrix multiplication and applies an elementwise activation function $g(\cdot)$:

$$\mathbf{z}(\mathbf{x}) = g^{(1)}\left(\mathbf{W}^{(1)}\mathbf{x}\right)$$
$$\mathbf{y}(\mathbf{x}) = g^{(2)}\left(\mathbf{W}^{(2)}\mathbf{z}(\mathbf{x})\right)$$

- Key step: *Now we also make the earlier layer learnable!*
- This is known as a Multi-Layer Perceptron (MLP).

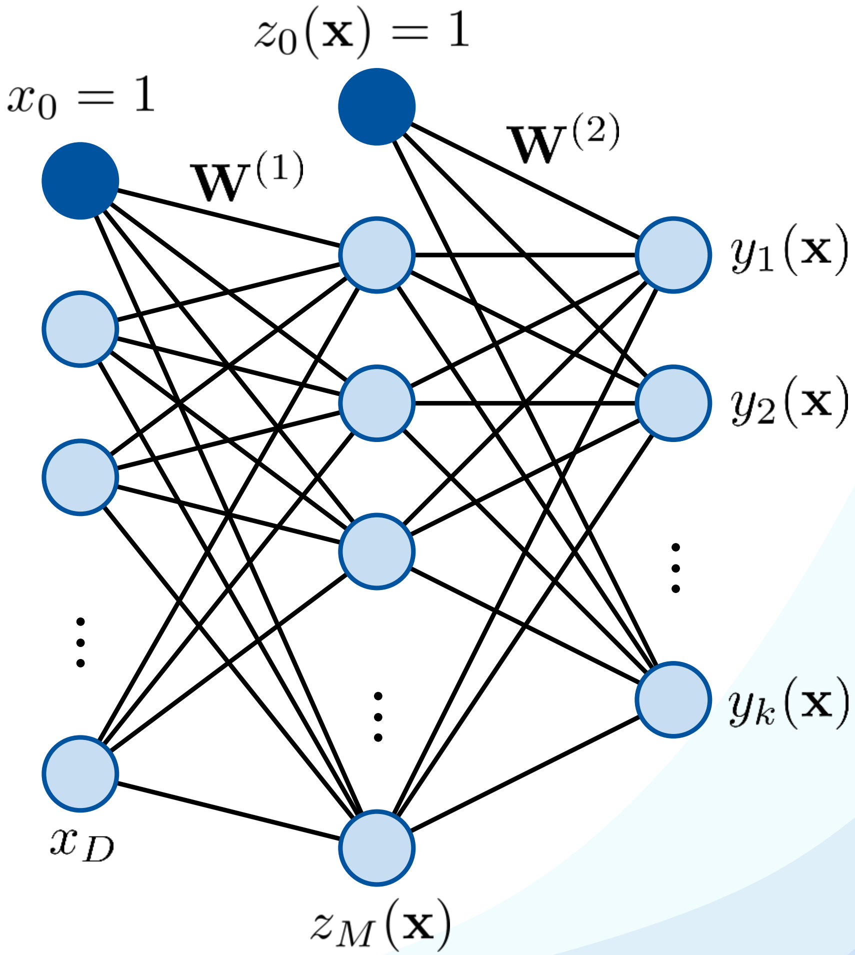


General Network Structure

- Multi-Layer Perceptron model:

$$y_k(\mathbf{x}) = g^{(2)}\left(\sum_{i=0}^{M} w_{ki}^{(2)} g^{(1)}\left(\sum_{j=0}^{D} w_{ij}^{(1)} x_j\right)\right)$$

- Usually, each layer adds a bias term.
- Activation functions between layers should be non-linear.
  - For example: $g^{(2)}(a) = \sigma(a),\ g^{(1)}(a) = \max\{a, 0\}$
  - With linear activations, successive layers would still compute a linear function.
- The hidden layer can have an arbitrary number of nodes.
- There can also be multiple hidden layers.

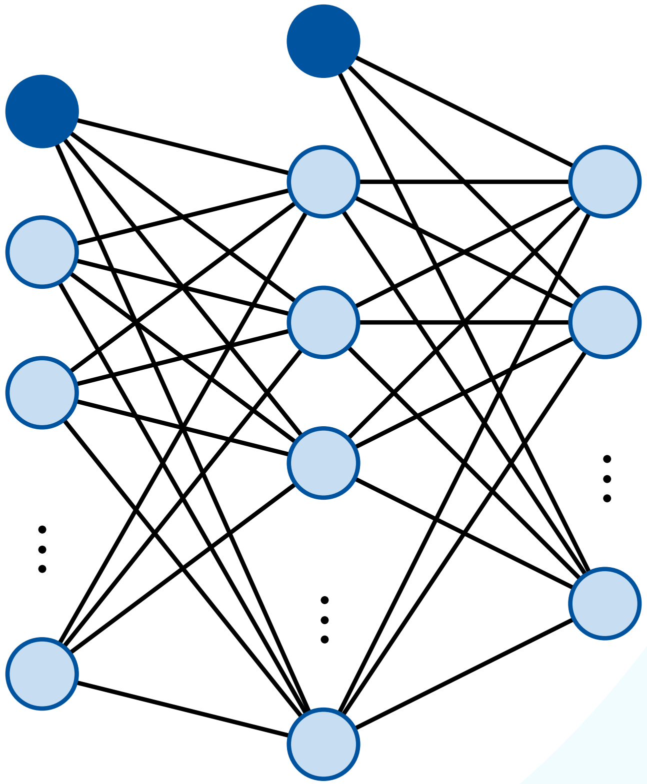


MLPs are Universal Approximators

$$y_k(\mathbf{x}) = g^{(2)}\left(\sum_{i=0}^{M} w_{ki}^{(2)} g^{(1)}\left(\sum_{j=0}^{D} w_{ij}^{(1)} x_j\right)\right)$$

- Universal Approximator Theorem:
  - A network with one hidden layer can approximate any continuous function of a compact domain arbitrarily well (assuming sufficient hidden nodes).

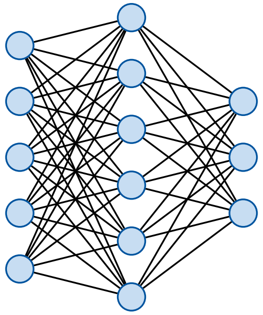
$\Rightarrow$ *Way more powerful than linear models!*



Learning with Hidden Units

- We now have a model that contains multiple layers of adaptive non-linear hidden units.
- How can we train such models?
  - Need to train *all* weights, not just last layer.
  - Learning the weights to the hidden units = learning features.
  - We don't know what the hidden units should do.
- Basic Idea: Gradient Descent.

This is the main challenge of deep learning!

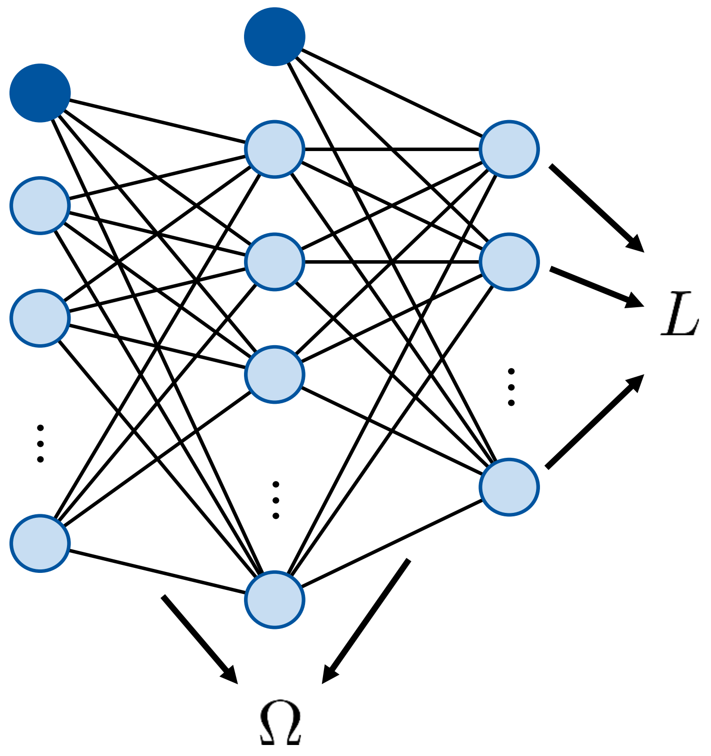


$E(\mathbf{w})$ → $\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$ → $\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$ → Repeat until convergence.

Apply Error Function | Calculate Gradients | Update Weights

Neural Network Basics

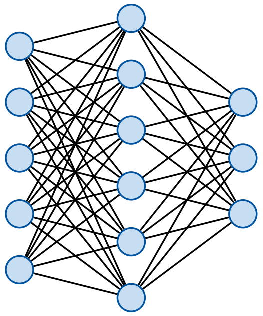
1. Perceptrons
2. Multi-Layer Perceptrons
3. **Loss Functions**
4. Backpropagation
5. Stochastic Gradient Descent



Loss Functions

- We train Neural Networks by minimizing an error function
  - In principle, any differentiable objective function can be used here.
  - Typically, we use a combination of a loss function $L(t, y(\mathbf{x}))$ and a regularizer $\Omega(\mathbf{w})$:

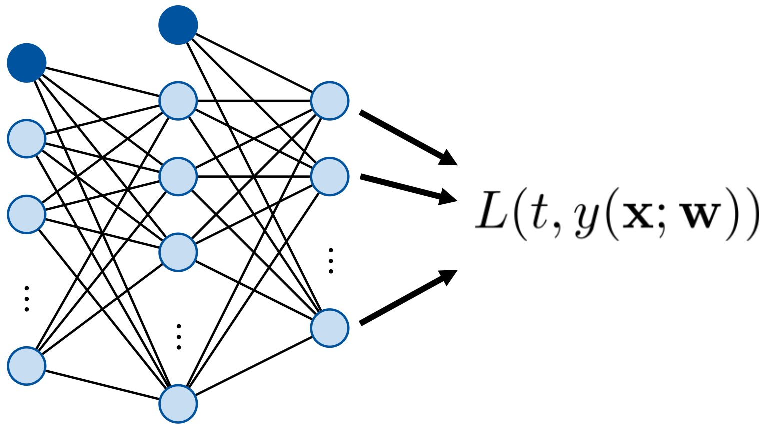
$$E(\mathbf{w}) = \sum_{n=1}^{N} L(t_n, y(\mathbf{x}_n; \mathbf{w})) + \lambda \Omega(\mathbf{w})$$



$E(\mathbf{w})$ → $\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$ → $\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$

Apply Error Function | Calculate Gradients | Update Weights

Examples of Loss Functions



- We can use any of the loss functions we have seen so far to achieve different effects:
  - L_2 loss (Squared Error)

    $$L(t, y(\mathbf{x})) = \frac{1}{2}(y(\mathbf{x}) - t)^2$$

    $\Rightarrow$ Least-squares regression / classif.
  - Binary Cross-Entropy loss

    $$L(t, y(\mathbf{x})) = -(t \ln \sigma(y(\mathbf{x})) + (1-t)\ln(1 - \sigma(y(\mathbf{x}))))$$

    $\Rightarrow$ Logistic regression
  - Hinge loss

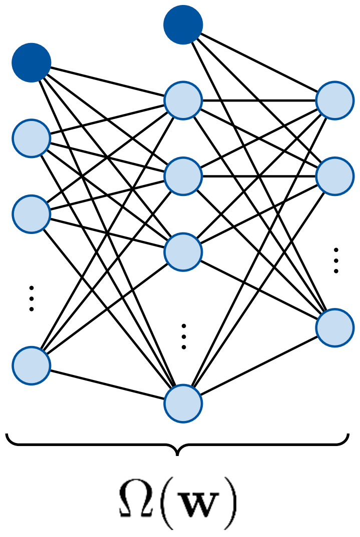
    $$L(t, y(\mathbf{x})) = [1 - t y(\mathbf{x})]_+$$

    $\Rightarrow$ SVM classification
  - Multi-Class Cross-Entropy loss

    $$L(t, \mathbf{y}(\mathbf{x})) = -\sum_k \left(\mathbb{I}(t = k) \ln \frac{\exp(y_k(\mathbf{x}))}{\sum_j \exp(y_j(\mathbf{x}))} \right)$$

    $\Rightarrow$ Multi-class probabilistic classification

Examples of Regularization Terms



- Similarly, we can use any of the regularization terms we have seen so far:
  - L_2 regularizer ("Weight Decay")

$$\Omega(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_2^2$$

  - L_1 regularizer

$$\Omega(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_1$$

$\Rightarrow$ Prevents overfitting

$\Rightarrow$ Enforces sparsity (feature selection)

- Since Neural Networks have many parameters, regularization becomes an important consideration.
  - Many of the more advanced NN "training tricks" can also be understood as a form of regularization

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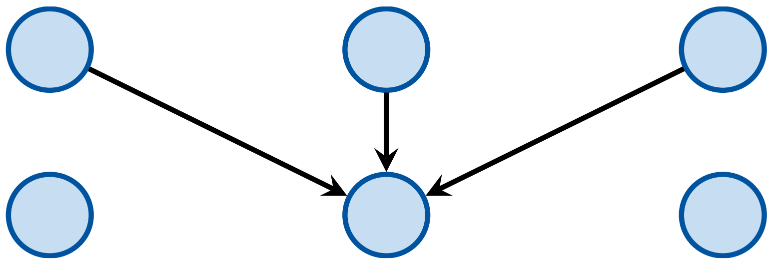
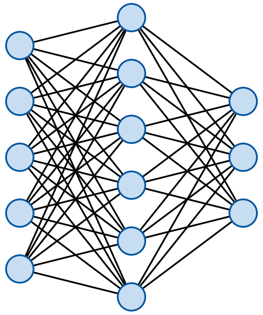


Backpropagation

- We know a flexible model that is able to learn features.
- We also know how to compute an error estimate.
- Now we need to compute the gradients with respect to our parameters.



$E(\mathbf{w})$

Apply Error Function

$\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$

Calculate Gradients

?

$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$

Update Weights

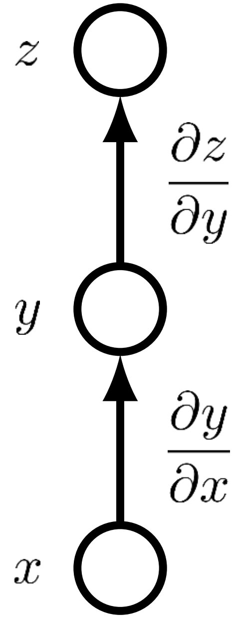
Approach 1: Naïve Analytical Differentiation

- Compute the gradients of each variable analytically.
- Scalar case is straightforward:

$$\Delta z = \frac{\partial z}{\partial y} \Delta y \qquad \Delta y = \frac{\partial y}{\partial x} \Delta x$$

$$\Delta z = \frac{\partial z}{\partial y} \frac{\partial y}{\partial x} \Delta x$$

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \frac{\partial y}{\partial x}$$

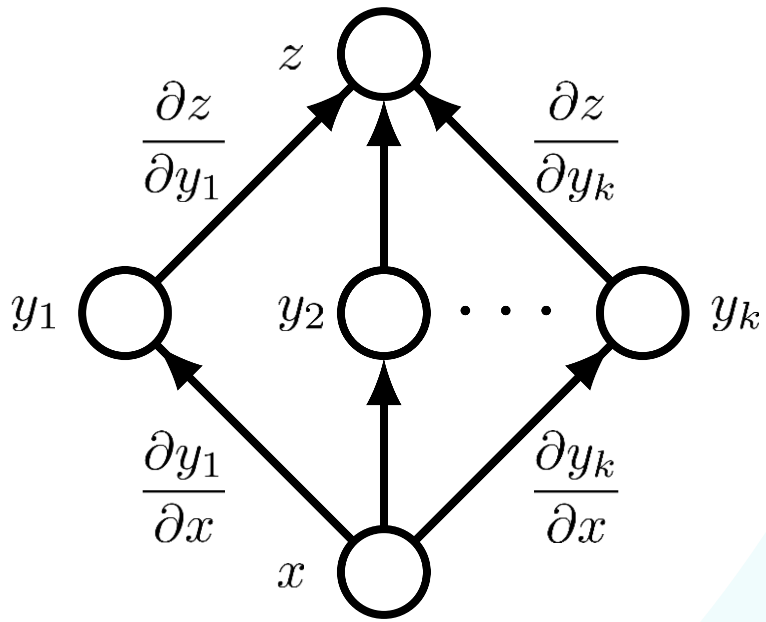


Approach 1: Naïve Analytical Differentiation

- Compute the gradients of each variable analytically.
- Scalar case is straightforward.
- Multi-dimensional case: Total derivative
  - Need to sum over all paths to target variable:

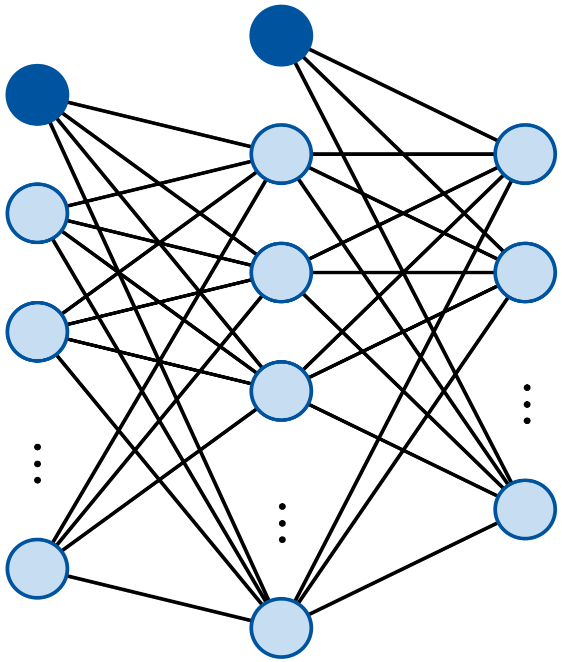
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x} + \ldots = \sum_{i=1}^{k} \frac{\partial z}{\partial y_i}\frac{\partial y_i}{\partial x}$$

  - With increasing depth, there will be exponentially many paths!



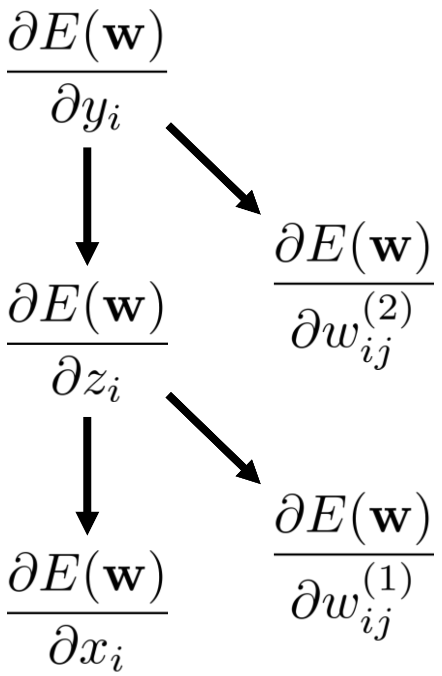
Approach 2: Numerical Differentiation

- Given the current state $\mathbf{w}^{(\tau)}$, we can evaluate $E(\mathbf{w}^{(\tau)})$.
- Idea: Make small changes to $\mathbf{w}^{(\tau)}$ and accept those that improve $E(\mathbf{w}^{(\tau)})$.
- Need several forward passes for each weight – over the whole dataset.
- This is horribly inefficient!

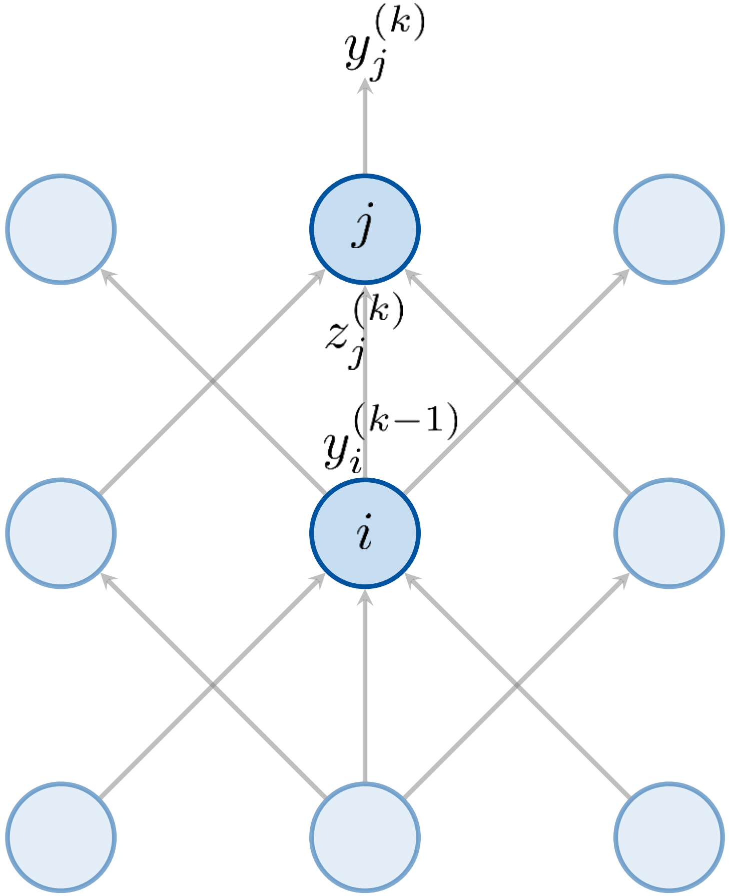


Approach 3: Incremental Analytical Differentiation

- Idea: compute the gradients layer by layer.
- Each layer below builds upon the results of the layer above.
- The gradient is propagated backwards through the layers.
- This is the backpropagation algorithm.



Example: Backpropagation for MLPs



$$\frac{\partial E}{\partial z_j^{(k)}} = \frac{\partial y_j^{(k)}}{\partial z_j^{(k)}} \frac{\partial E}{\partial y_j^{(k)}} = \frac{\partial g\left(z_j^{(k)}\right)}{\partial z_j^{(k)}} \frac{\partial E}{\partial y_j^{(k)}}$$

$$\frac{\partial E}{\partial y_i^{(k-1)}} = \sum_j \frac{\partial z_j^{(k)}}{\partial y_i^{(k-1)}} \frac{\partial E}{\partial z_j^{(k)}}$$

Input of layer k: $z_j^{(k)} = \sum_i w_{ji}^{(k-1)} y_i^{(k-1)}$

Output of layer k: $y_j^{(k)} = g\left(z_j^{(k)}\right)$

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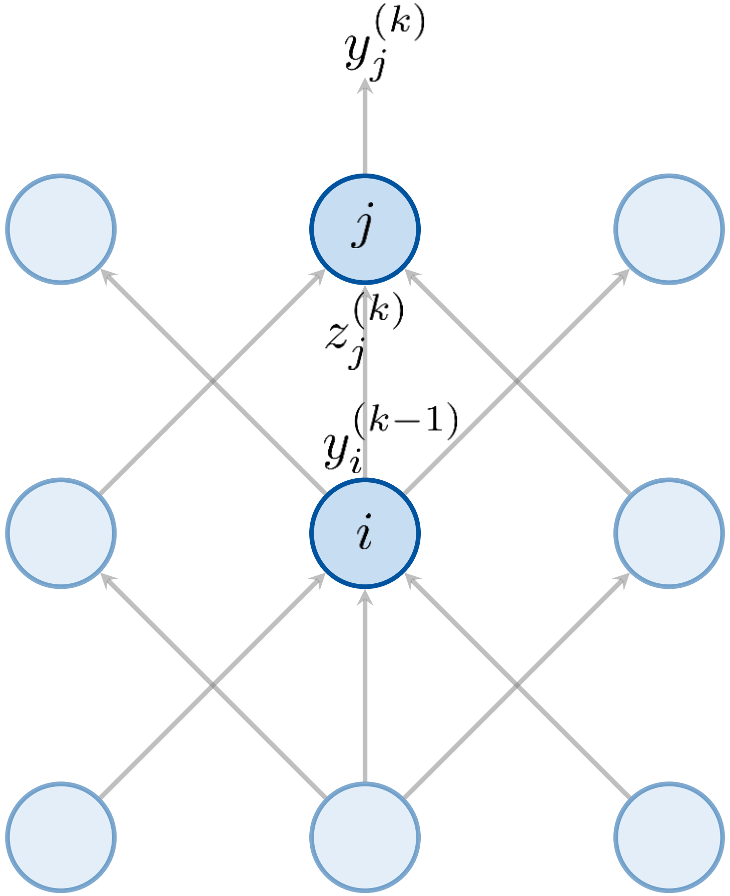

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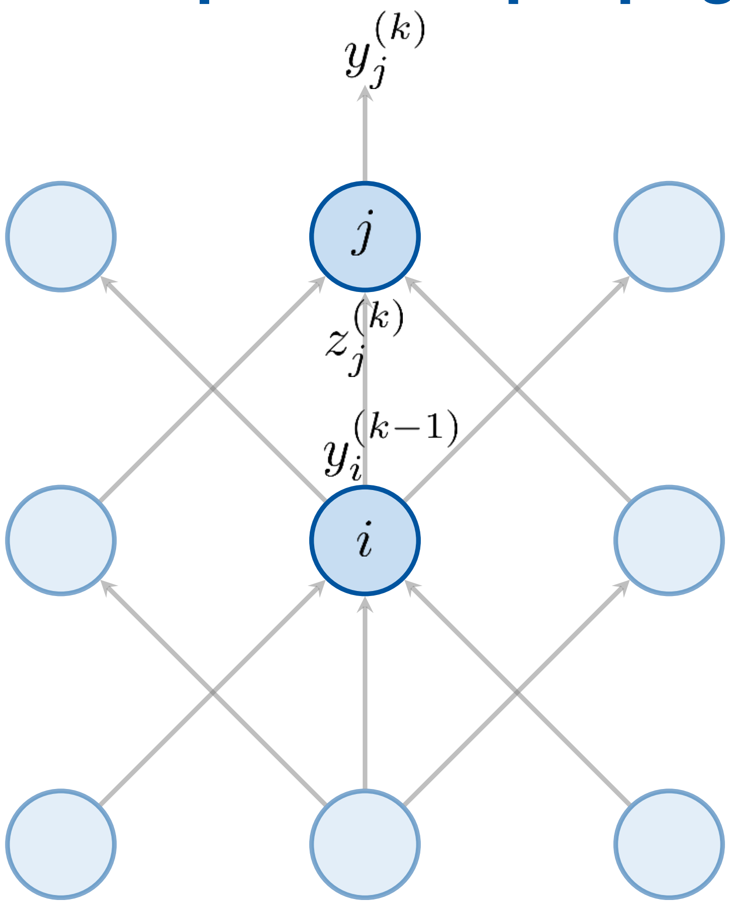

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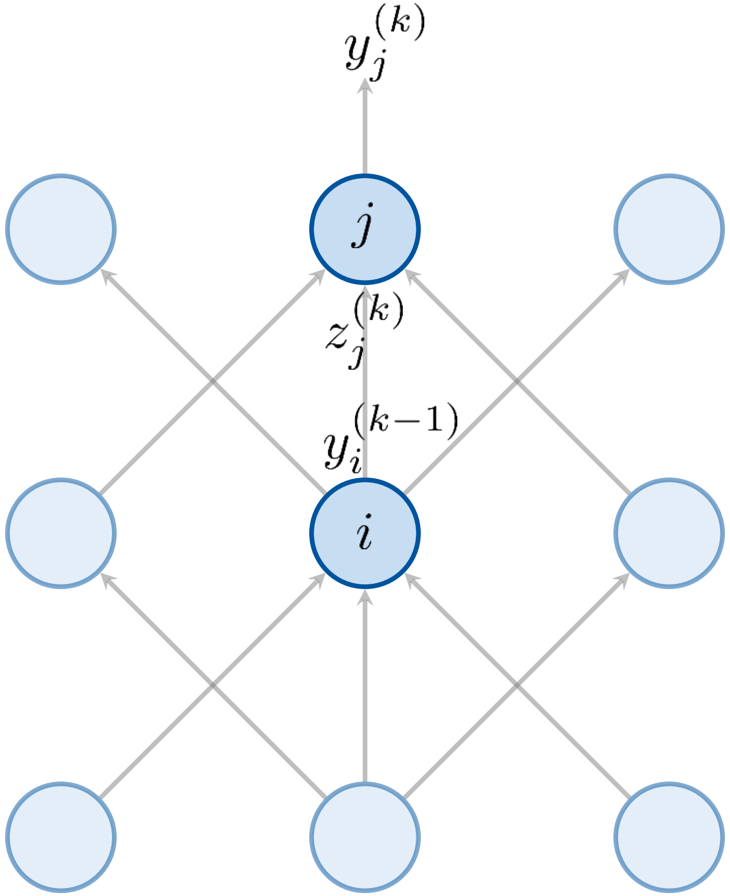

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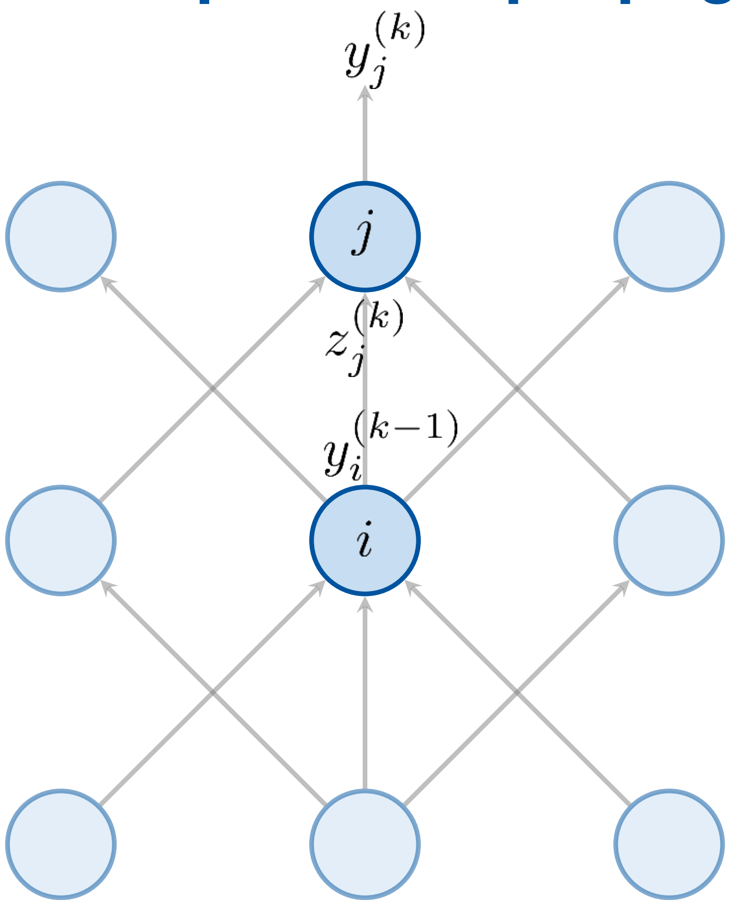

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Discussion Backpropagation

Advantages

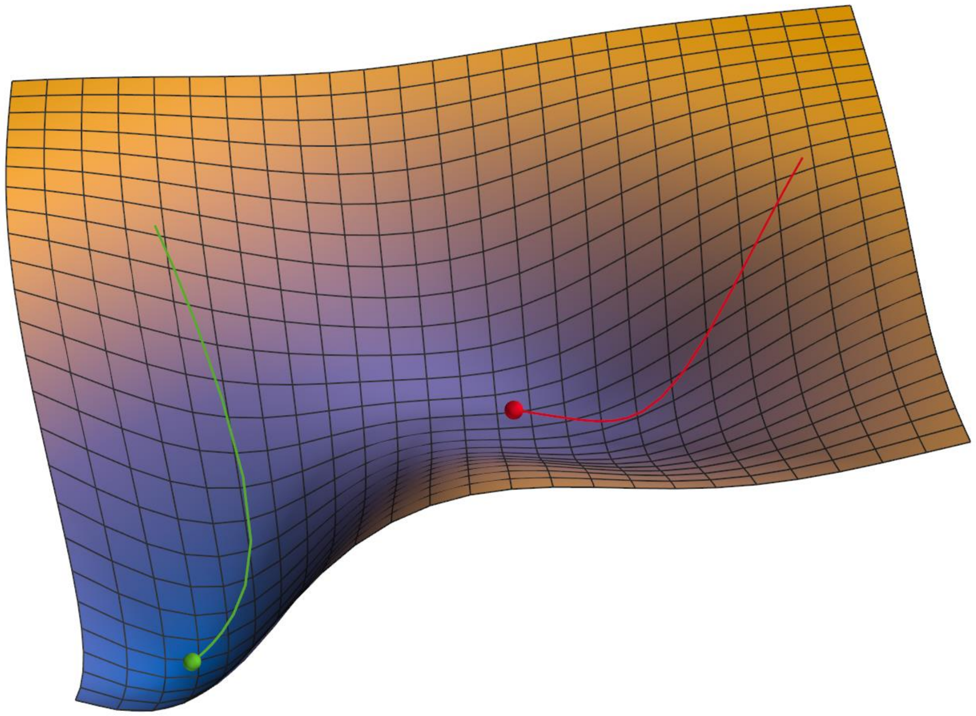
- Very general algorithm, widely used.
- Efficiently computes all gradients in the network using dynamic programming.
- The same concept can be applied to any differentiable function.
  - This makes it possible to define other types of layers.

Limitations

- Efficient evaluation of backpropagation requires storing all unit activations from forward pass.
  - The amount of memory necessary for this imposes a practical limit on the size of the network.
- Successful learning relies on the gradients to be propagated to the early network layers.
  - Numerical challenges may arise here.

Neural Network Basics

1. Perceptrons
2. Multi-Layer Perceptrons
3. Loss Functions
4. Backpropagation
5. **Stochastic Gradient Descent**

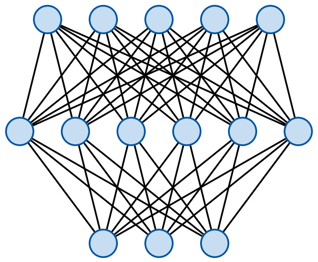


Stochastic Gradient Descent

- Now that we have the gradients, we need to update the weights.
- We already know the basic equation for this
  - (1st-order) Gradient Descent

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

- Remaining Questions:
  - On what data do we want to apply this?
  - How should we choose the learning rate η ?



Apply Error Function

Calculate Gradients

Update Weights

Stochastic vs. Batch Learning

- Batch Learning
  - Process the full dataset in one batch.
  - Compute the gradient based on all training examples.

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

- Stochastic Learning
  - Choose a single example from the training set.
  - Compute the gradient only based on this example.
  - This estimate will generally be noisy, which has some advantages.

$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

Batch Learning

- Conditions of convergence are well understood.
- Many acceleration techniques only work in batch learning.
- Theoretical analysis of the weight dynamics and convergence rates are simpler.

Stochastic Learning

- Usually much faster than batch learning.
- Often results in better solutions.
- Can be used for tracking changes when the target distribution shifts.

Middle ground: Minibatches

Minibatches

- Idea
  - Process only a small batch of training examples together.
  - Start with a small batch size & increase it as training proceeds.

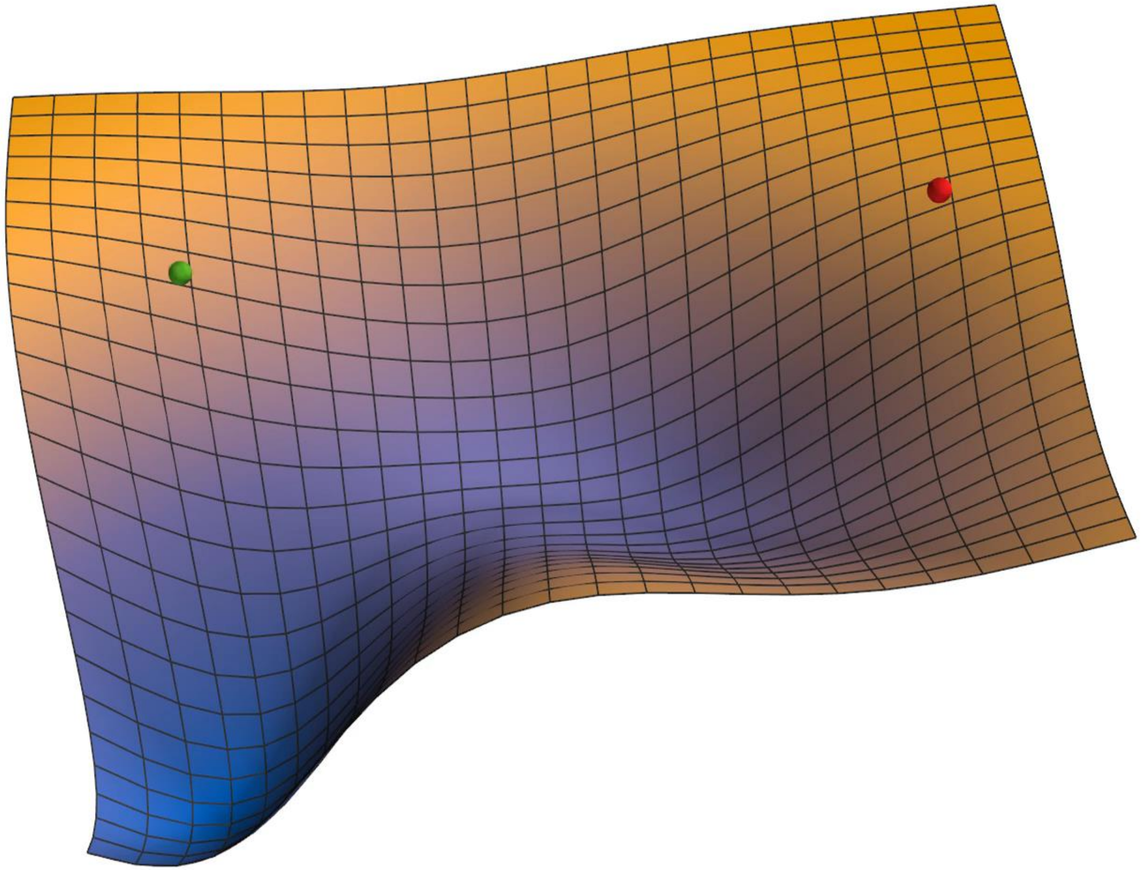
$$\mathcal{B} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_B, t_B)\} \subset \mathcal{D}$$

- Advantages
  - Gradients will be more stable than for stochastic gradient descent, but still faster to compute than with batch learning.
  - Take advantage of redundancies in the training set.
  - Matrix operations are more efficient than vector operations.

- Caveat
  - Need to normalize error function by the minibatch size to use the same learning rate between minibatches

$$E(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} L(t_n, y(\mathbf{x}_n; \mathbf{w})) + \frac{\lambda}{N} \Omega(\mathbf{w})$$

Example



Choosing the Right Learning Rate

- Consider a simple 1D example:

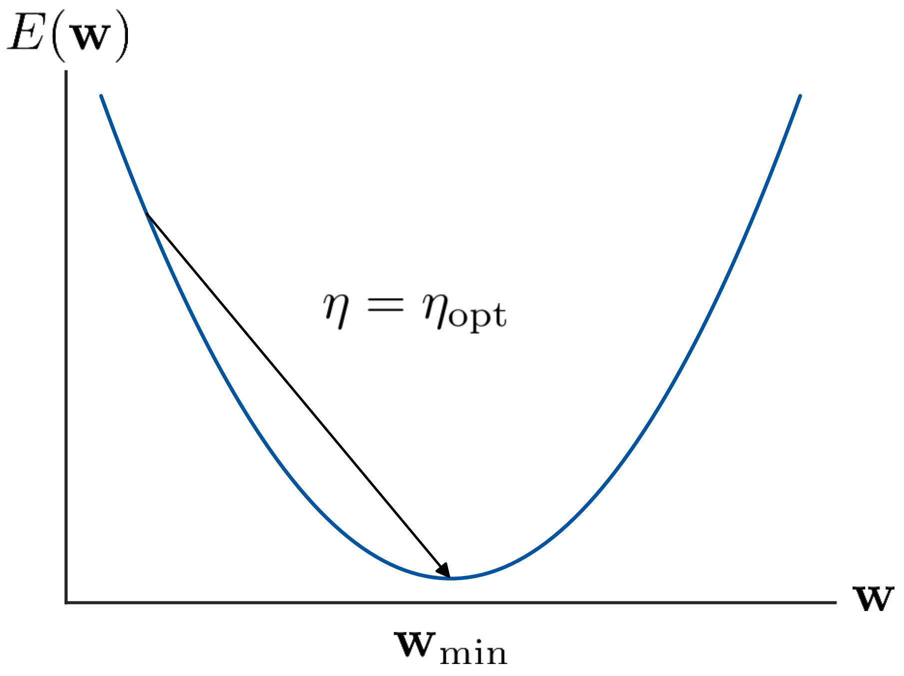
$$w^{(\tau+1)} = w^{(\tau)} - \eta \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$$

- What is the optimal learning rate η_{opt}?

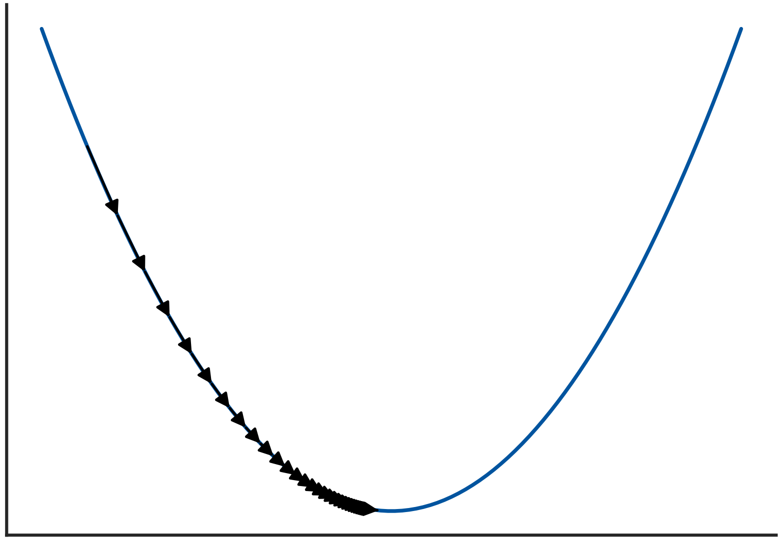
- If E is quadratic, the optimal learning rate is given by the inverse of the Hessian:

$$\eta_{\mathrm{opt}} = \left(\frac{\partial^2 E(\mathbf{w}^{(\tau)})}{\partial \mathbf{w}^2} \right)^{-1}$$

- *For neural networks, the Hessian is usually infeasible to compute.*

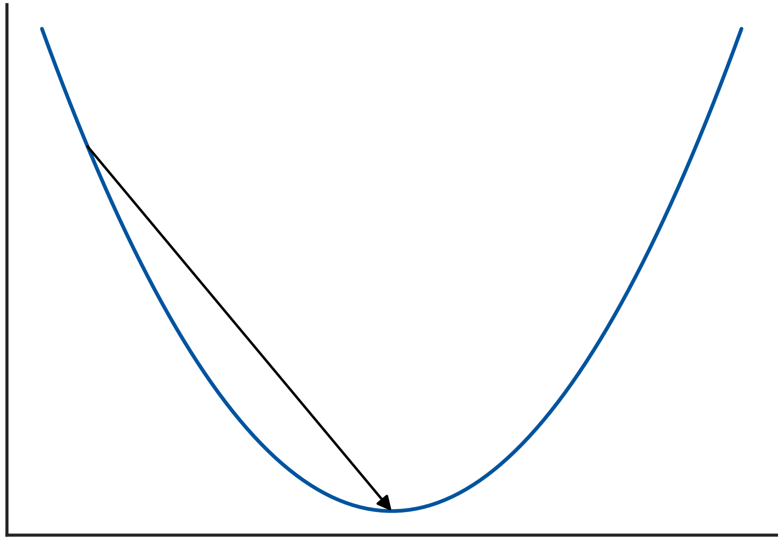


η too small



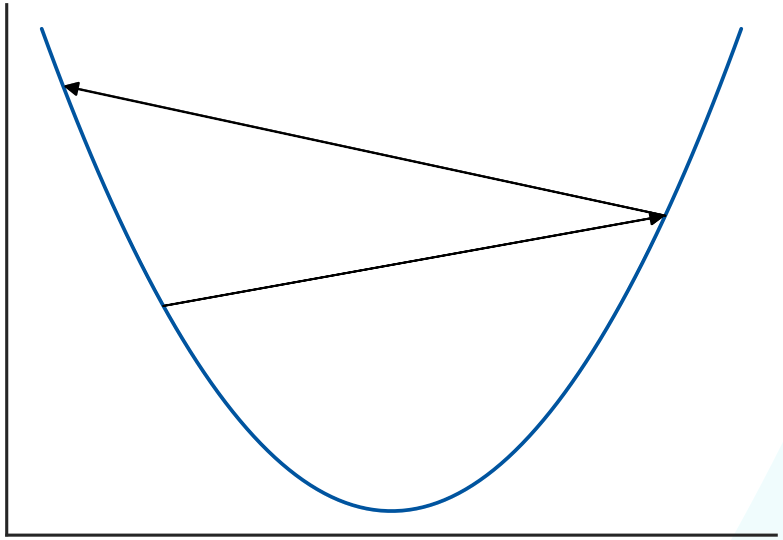
Convergence is slow

η_{opt}



Converges ideally in a single step

η too large



Might not converge

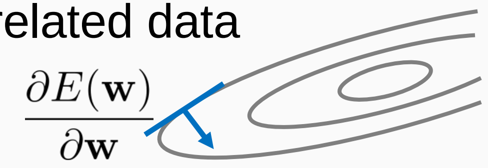
Discussion: Stochastic Gradient Descent

Advantages

- Very simple, but still quite robust method.
- Minibatches offer a compromise between stability and faster computation.
- Stochasticity in minibatches is often beneficial for learning

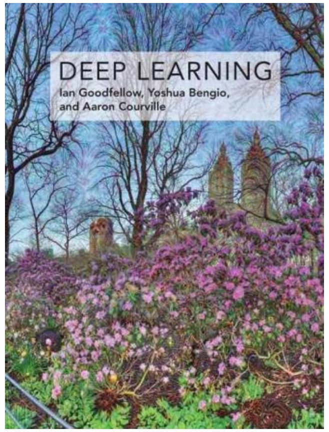
Limitations

- Finding a good setting for the learning rate is very important for fast convergence.
  - Choosing the right learning rate is a challenge and requires experience.
  - A different learning rate may be optimal for different parts of the network
- Following the direction of steepest descent is not always the fastest way to the optimum
  - E.g., in highly correlated data



References and Further Reading

- More information about Neural Networks and Deep Learning is available in the following book.



I. Goodfellow, Y. Bengio, A. Courville
Deep Learning
MIT Press, 2016

https://www.deeplearningbook.org/