SPATIAL ECOLOGY

Perceptron

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Agenda

1) The “less optimal” hyperplane methods

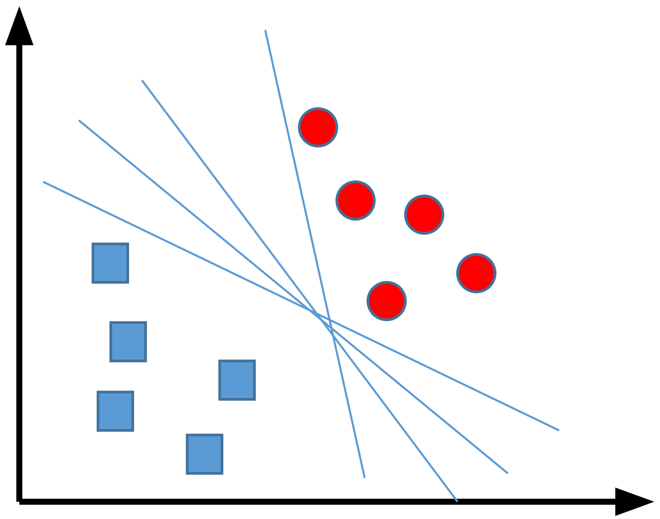
- Links between SVM and Logistic Regression
- Review on Linear Regression
- Minimizing loss functions
- Regularization

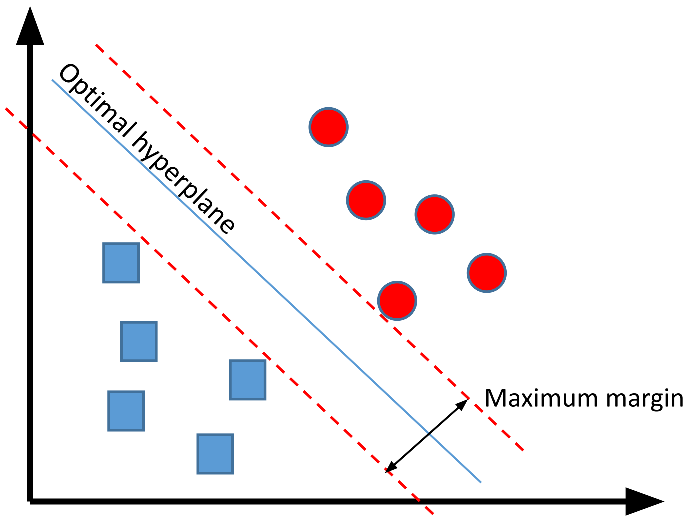
2) Perceptron

- The universal approximator
- Intro to optimizers
- Hands-on tutorial

Support Vector Machine

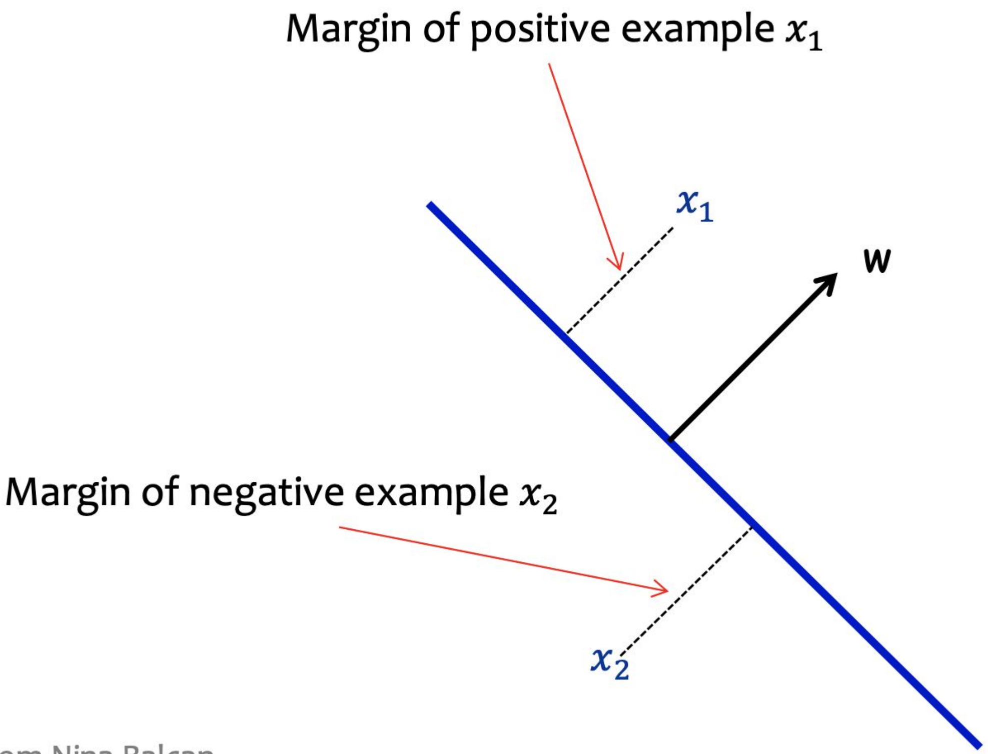
Find the optimal hyperplane in an N-dimensional space that distinctly classifies the data points.

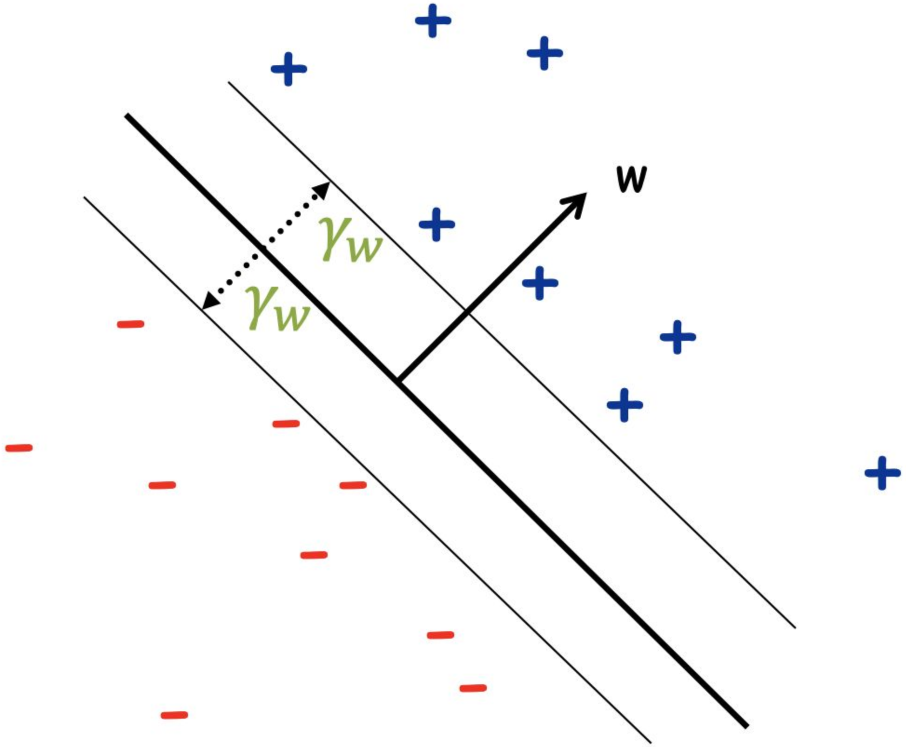




Geometric Margin

Definition: The margin of example x w.r.t. a linear sep. w is the distance from x to the plane





Slide from Nina Balcan

SVM Optimization

Hinge loss function

$$c(x, y, f(x)) = \begin{cases} 0, & \text{if } y * f(x) \geq 1 \\ 1 - y * f(x), & \text{else} \end{cases}$$

Loss function for the SVM

$$min_w \lambda \parallel w \parallel^2 + \sum_{i=1}^{n} (1 - y_i \langle x_i, w \rangle)_+$$

Gradients

$$\frac{\delta}{\delta w_k} \lambda \parallel w \parallel^2 \quad = 2\lambda w_k$$

$$\frac{\delta}{\delta w_k} \big(1 - y_i \langle x_i, w \rangle\big)_+ \quad = \begin{cases} 0, & \text{if } y_i \langle x_i, w \rangle \geq 1 \\ -y_i x_{ik}, & \text{else} \end{cases}$$

Updating the weights:

No misclassification

$$w = w - \alpha \cdot (2\lambda w)$$

Misclassification

$$w = w + \alpha \cdot (y_i \cdot x_i - 2\lambda w)$$

SVM for Regression

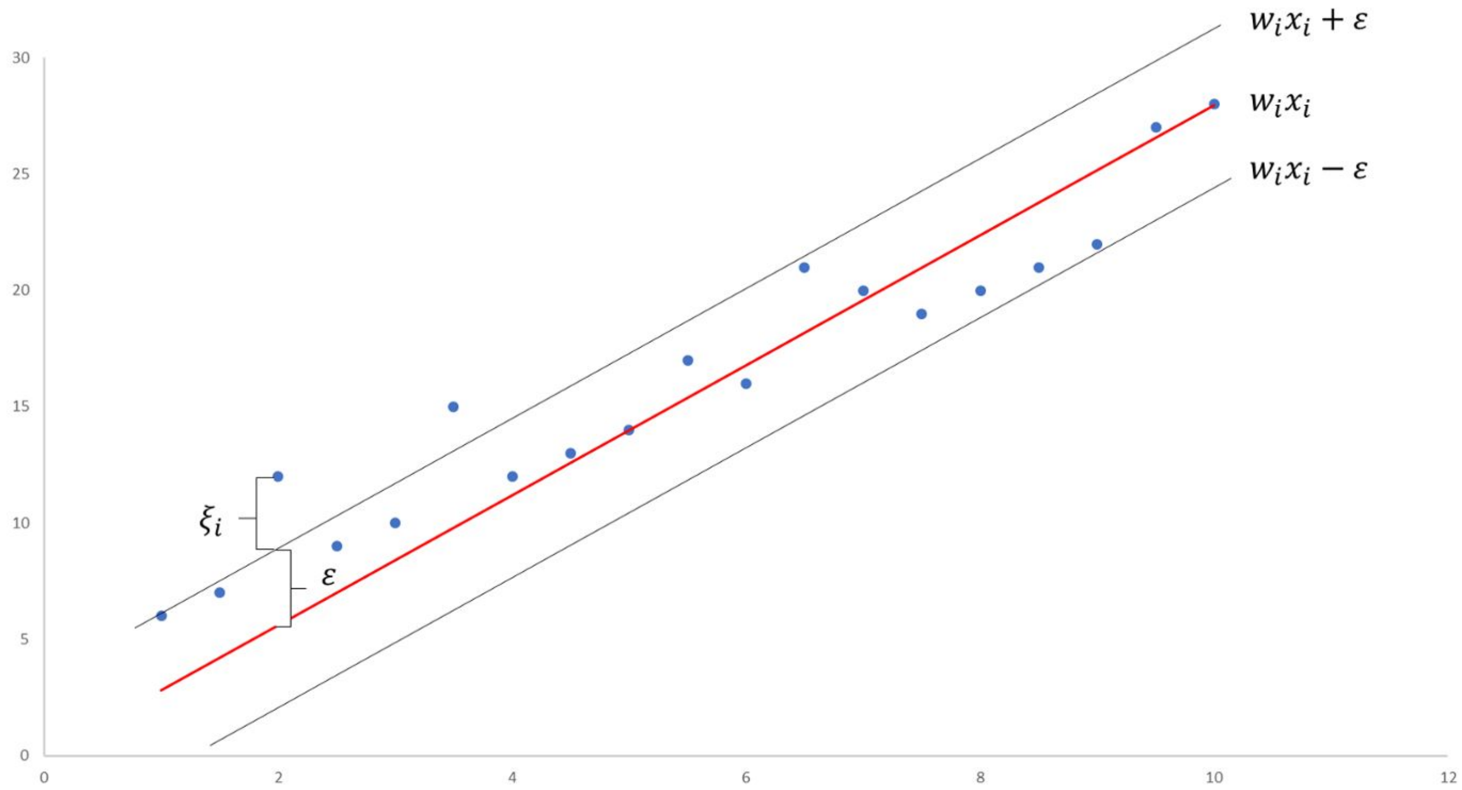
For any value that falls outside of ϵ, we can denote its deviation from the margin as ξ.

Loss

$$MIN\ \frac{1}{2}||\boldsymbol{w}||^2 + C\sum_{i=1}^{n}|\xi_i|$$

Constraints

$$|y_i - w_i x_i| \le \varepsilon + |\xi_i|$$



SVM for Regression

- The best fit line is the hyperplane that has the maximum number of points.
- Limitations
  - The fit time complexity of SVR is more than quadratic with the number of samples
  - SVR scales poorly with number of samples (e.g., >10k samples). For large datasets, **Linear SVR** or **SGD Regressor**
  - Underperforms in cases where the number of features for each data point exceeds the number of training data samples
  - Underperforms when the data set has more noise, i.e. target classes are overlapping.

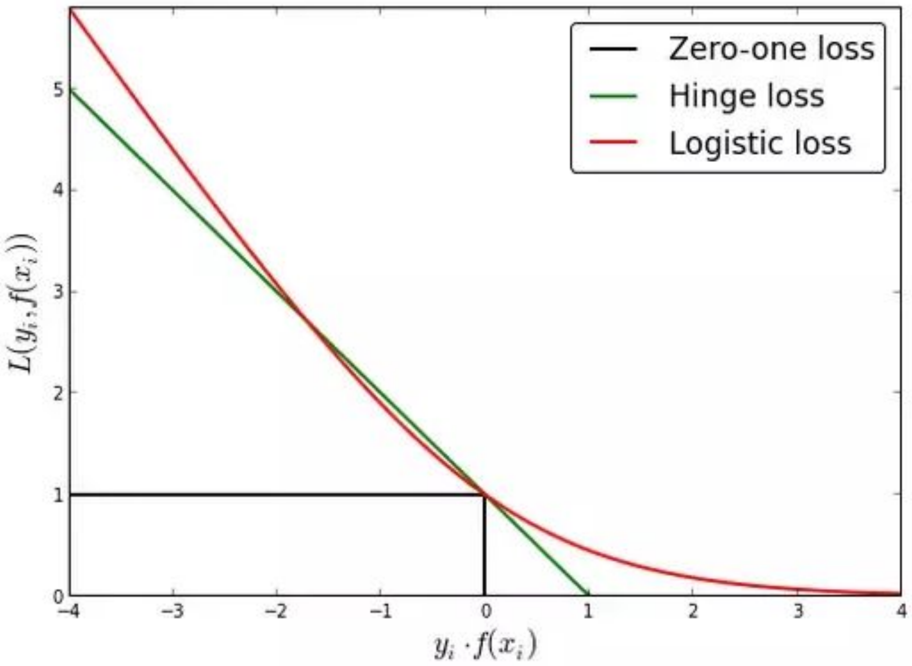
A “non-optimal” hyperplane approach

$$\min_w \lambda\|w\|^2 + \sum_i \max\{0, 1 - y_i w^T x_i\}$$ SVM

$$\min_w \lambda\|w\|^2 + \sum_i \log(1 + \exp(1 - y_i w^T x_i))$$ Logistic Regression (LR)

Main differences:

- SVM maximizes the margin between the closest support vectors
- LR maximizes the class probability
- SVM produces discrete classes (1 or 0)
- LR produces probabilistic values (sigmoid of the log likelihood function)



Review on Linear Regression

Task (T)

Input $x \in \mathbb{R}^n$

Weights $w \in \mathbb{R}^n$

$$\hat{y} = w^T x$$

$$f(x, w) = x_1 w_1 + x_2 w_2 + \cdots + x_n w_n$$

Performance (P)

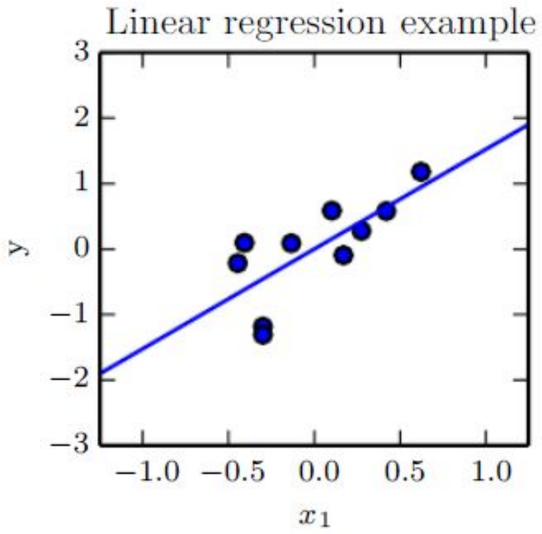
$$MSE_{test} = \frac{1}{m} \sum_i (\hat{y}_{test} - y_{test})_i^2$$

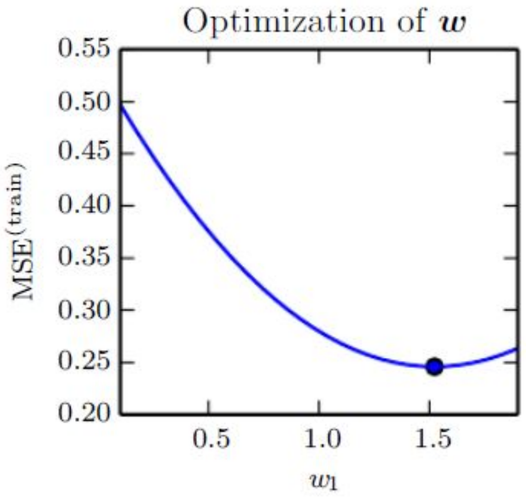
Dataset

$$(X, y) \left\{ \begin{array}{l} (X_{train}, y_{train}) \\ (X_{test}, y_{test}) \end{array} \right.$$

Training

$$\nabla_w \left(\frac{1}{m} \sum_i (w^T X_{train} - y_{train})_i^2 \right) = 0$$

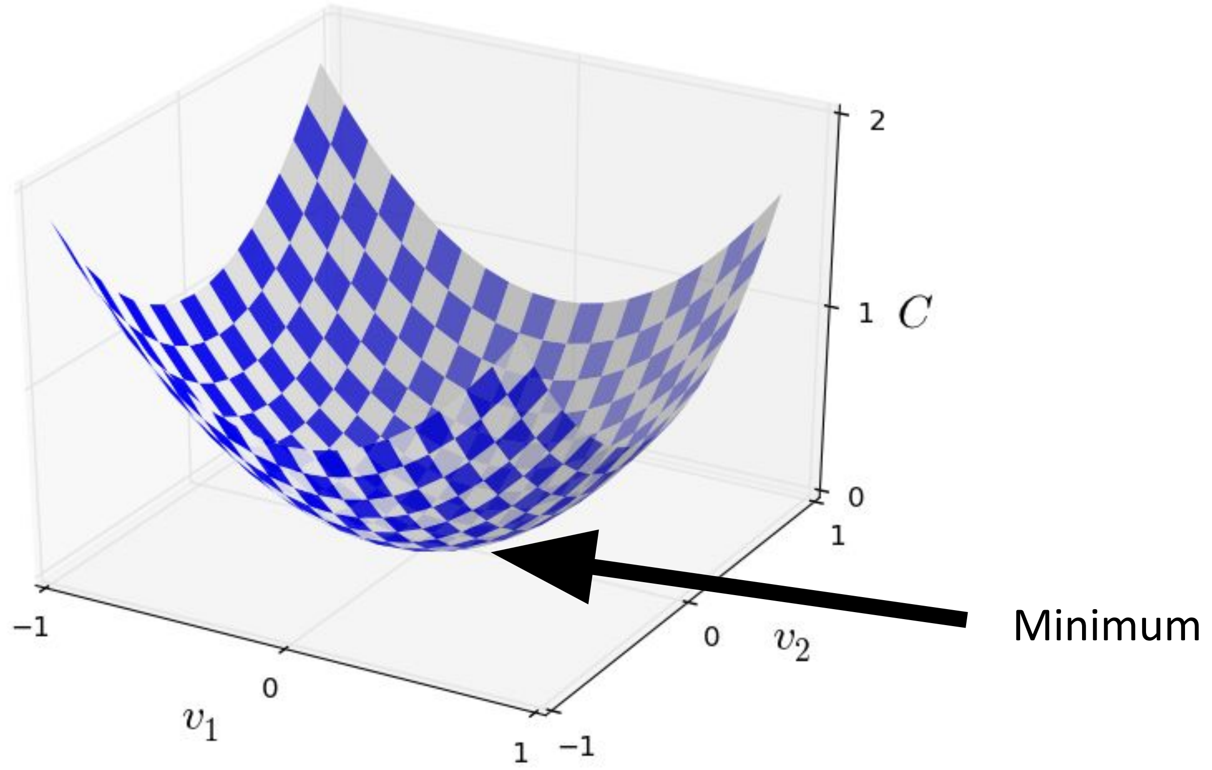




Solves linear problems

Can’t solve more complex problems (e.g., XOR problem)

Loss Minimization



Convex loss functions can be solved by differentiation, at the point where Loss is minimum the derivative wrt to parameters should be 0!

Linear Regression Optimization

- Add an offset w_0: $f(\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{w}^T \boldsymbol{x} + \mathrm{w}_0$, $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), \ldots (\boldsymbol{x}_n, y_n)\}$

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i + w_0 - y_i)^2$$

$$= \arg\min_{\boldsymbol{w}} L(\boldsymbol{w}; \mathcal{D})$$

- Set $\frac{\partial L(\boldsymbol{w};\mathcal{D})}{\partial w_i} = 0$ for each i

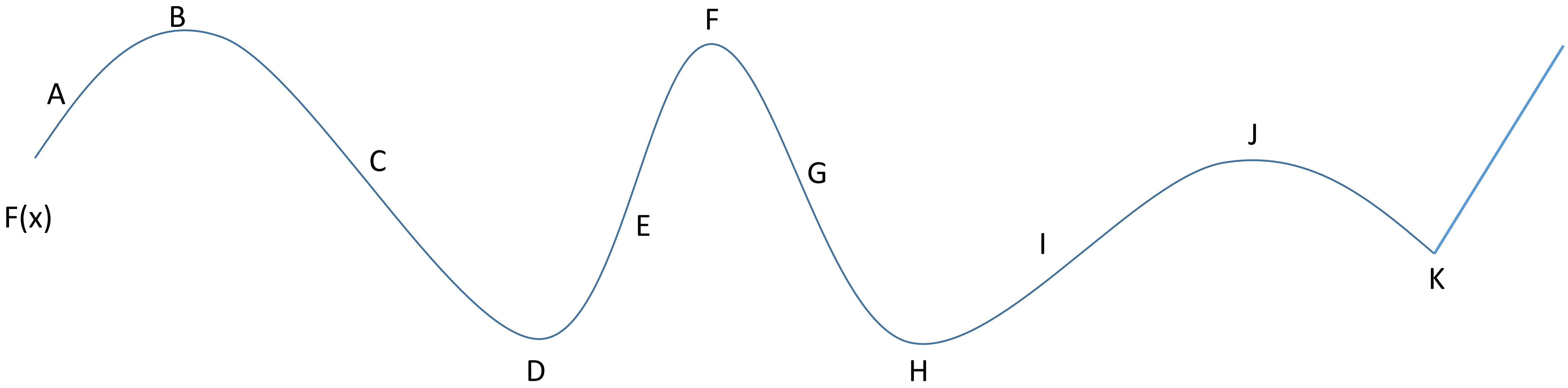
Mean squared error loss

Rewrite:

$$\begin{aligned}(X\mathbf{w}-\mathbf{y})^T(X\mathbf{w}-\mathbf{y}) &= (\mathbf{w}^TX^T-\mathbf{y}^T)(X\mathbf{w}-\mathbf{y}) \\ &= \mathbf{w}^TX^TX\mathbf{w}-\mathbf{w}^TX^T\mathbf{y}-\mathbf{y}^TX\mathbf{w}+\mathbf{y}^T\mathbf{y} \\ &= \mathbf{w}^TX^TX\mathbf{w}-2\mathbf{w}^TX^T\mathbf{y}+\mathbf{y}^T\mathbf{y}.\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial w}\mathbf{w}^TX^TX\mathbf{w}-2\mathbf{w}^TX^T\mathbf{y}+\mathbf{y}^T\mathbf{y} &= 0 \\ 2X^TX\mathbf{w}-2X^T\mathbf{y} &= 0 \\ X^TX\mathbf{w} &= X^T\mathbf{y} \\ \mathbf{w} &= (X^TX)^{-1}X^T\mathbf{y}\end{aligned}$$

More on the derivatives



Regularization

- Ridge regression: penalize with L2 norm

$$\boldsymbol{w}^* = \arg\min \sum_i L(f(\boldsymbol{x}_i; \boldsymbol{w}), y_i) + \lambda \sum_{j=1}^{m} w_j^2$$

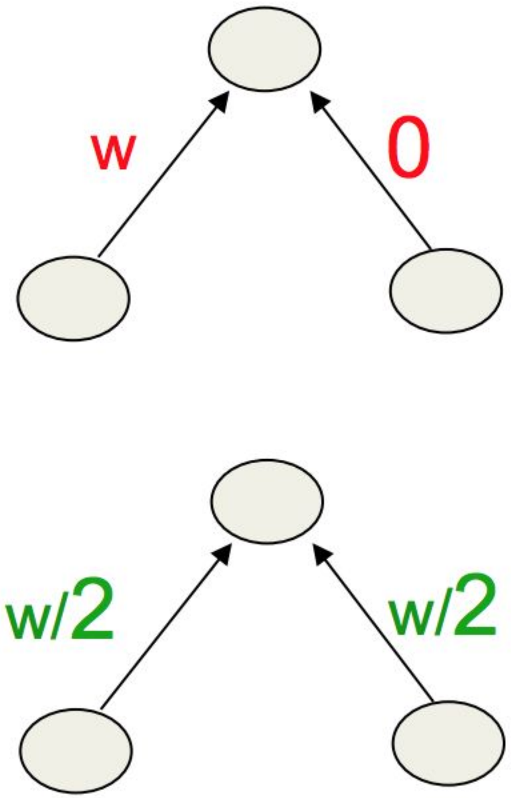
  - Closed form solution exists $\boldsymbol{w}^* = (\lambda I + X^T X)^{-1} X^T \boldsymbol{y}$

- LASSO regression: penalize with L1 norm

$$\boldsymbol{w}^* = \arg\min \sum_i L(f(\boldsymbol{x}_i; \boldsymbol{w}), y_i) + \lambda \sum_{j=1}^{m} |w_j|$$

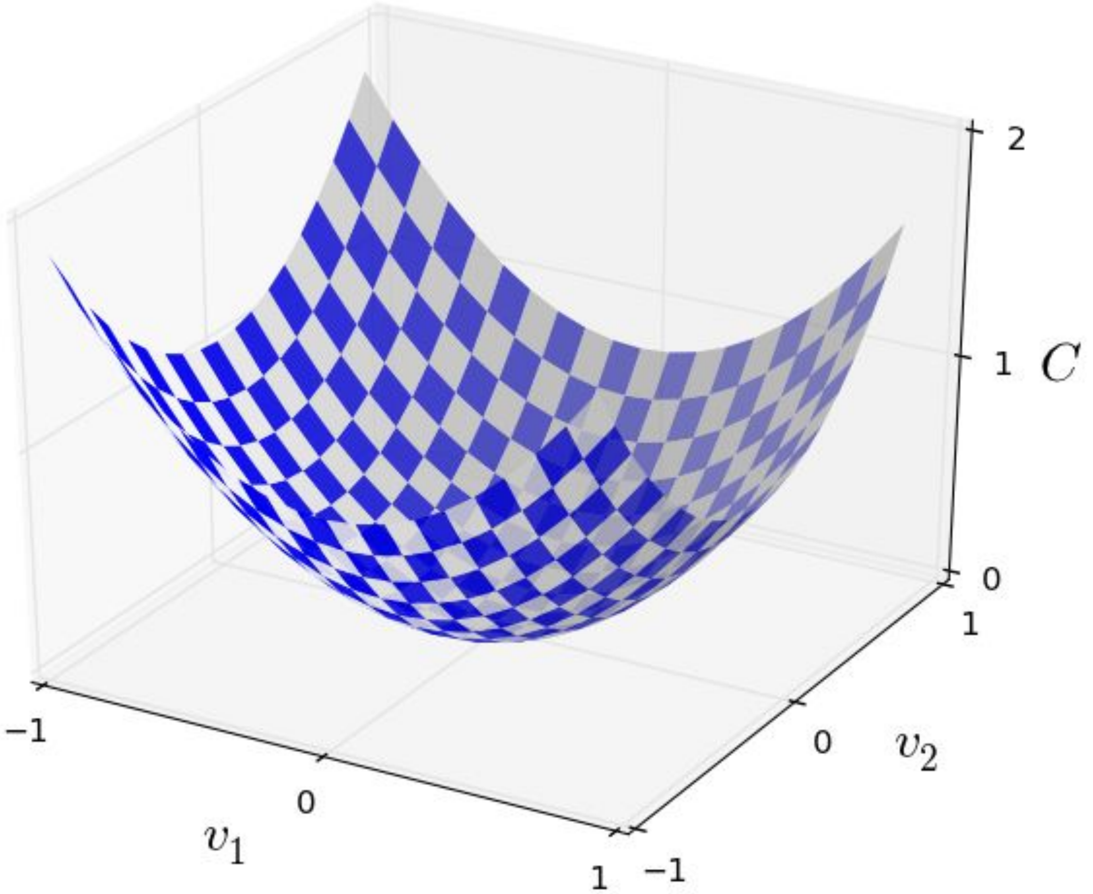
  - No closed form solution but still convex (optimal solution can be found)

Regularization

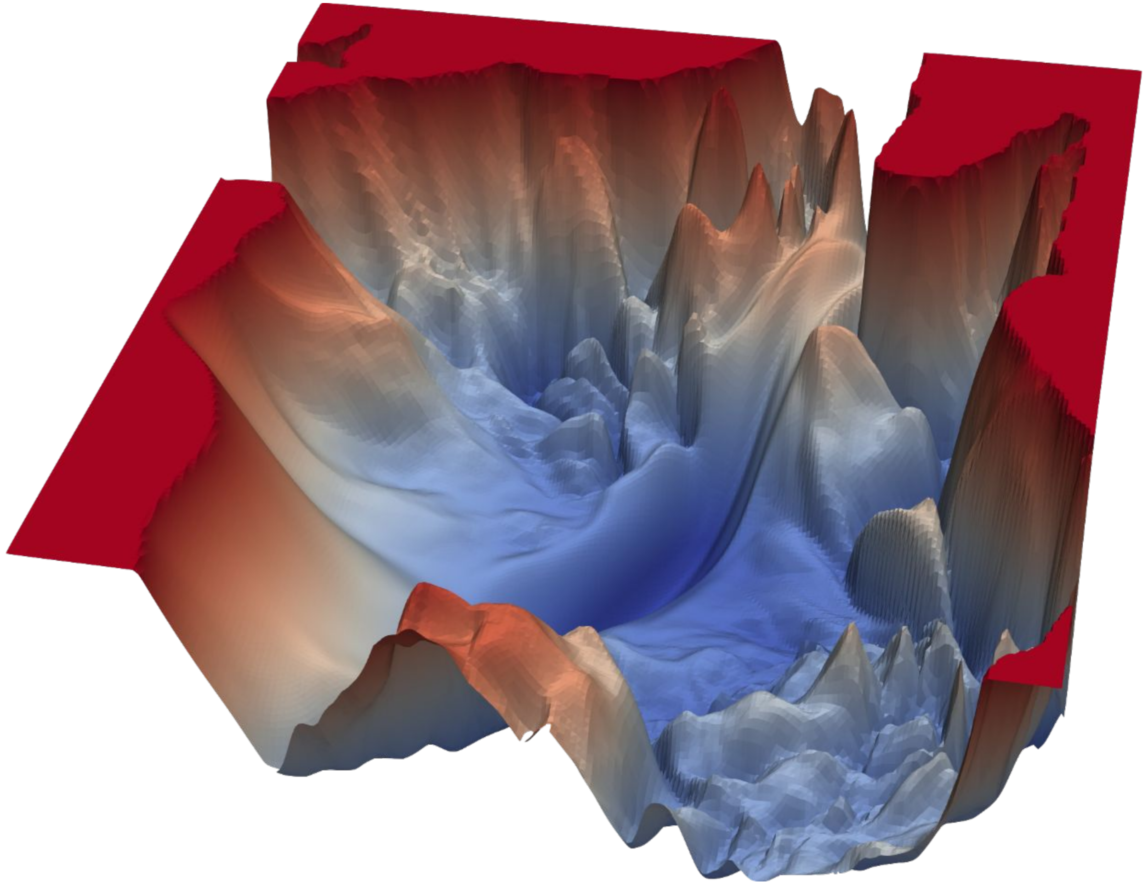


- Prefers to share smaller weights
- Makes model smoother
- More Convex

Expectation

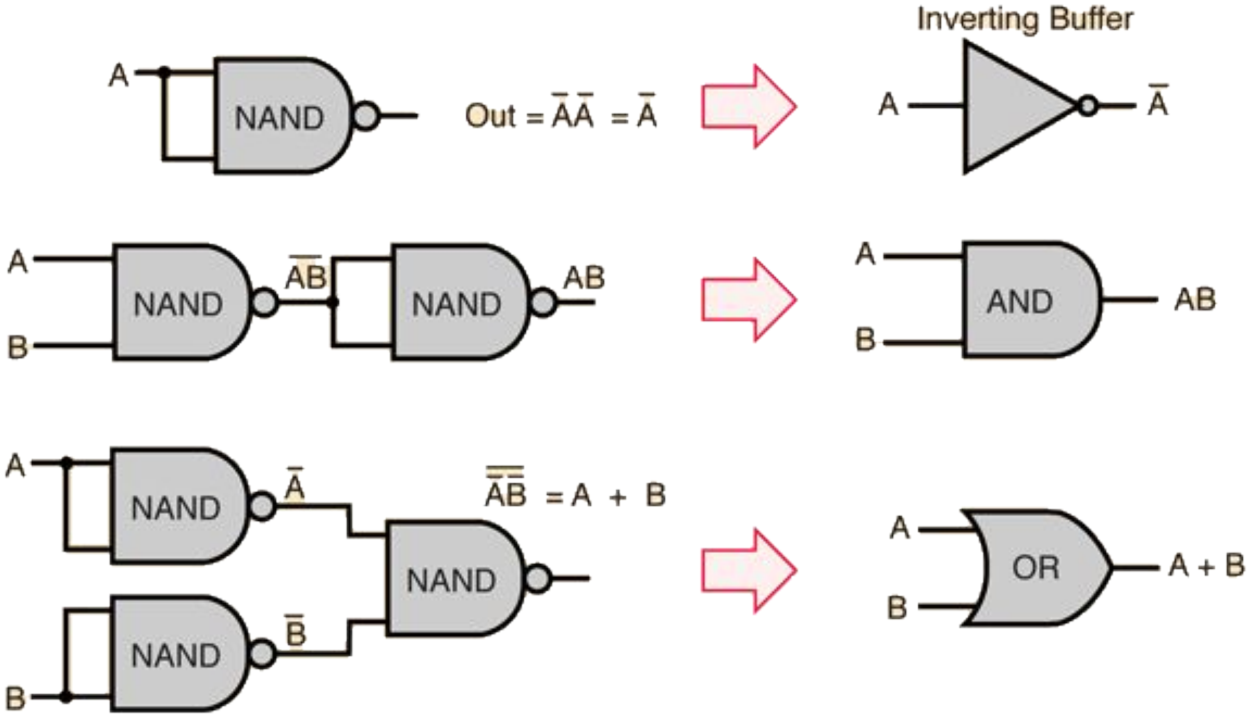


Reality



Logic circuits with perceptrons

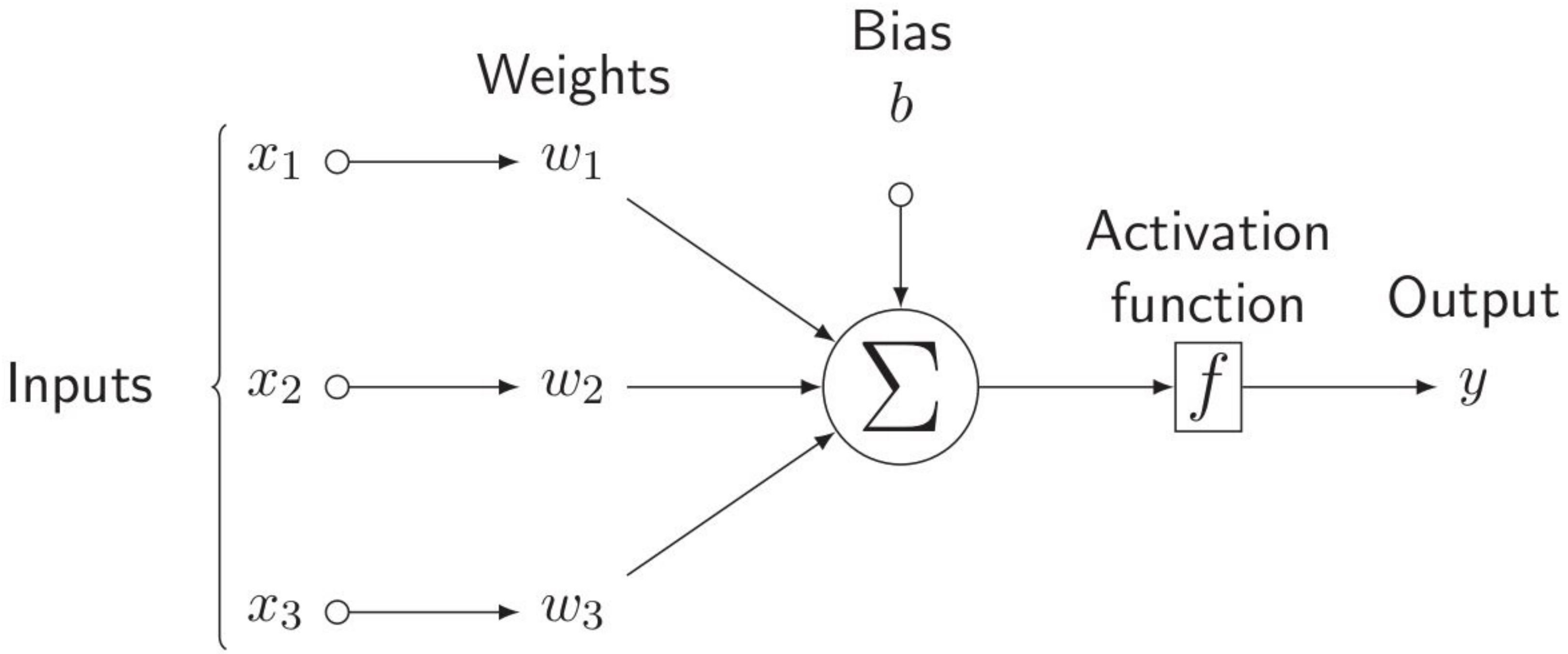
- NAND gates can be constructed from perceptrons
- NAND gates are universal for computation
  - Any computation can be built from NAND gates
  - Therefore, perceptrons are universal for computation



Nielsen, 2015

Perceptron: Threshold Logic

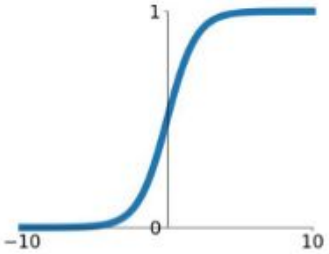
$$\mathcal{L}_{\text{perc}}(\mathbf{x}, y) = \begin{cases} 0 & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) > 0 \\ -y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) \le 0 \end{cases}$$



Activation functions

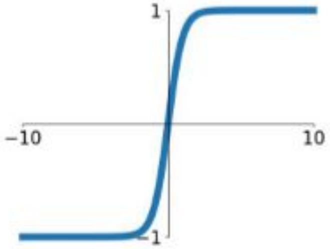
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



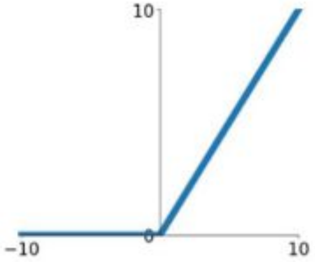
tanh

$\tanh(x)$



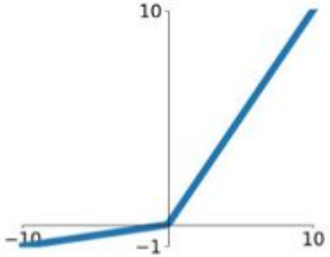
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

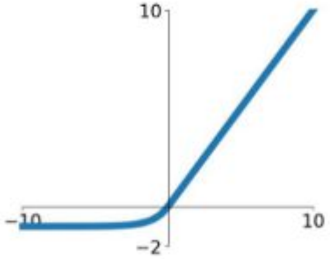


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



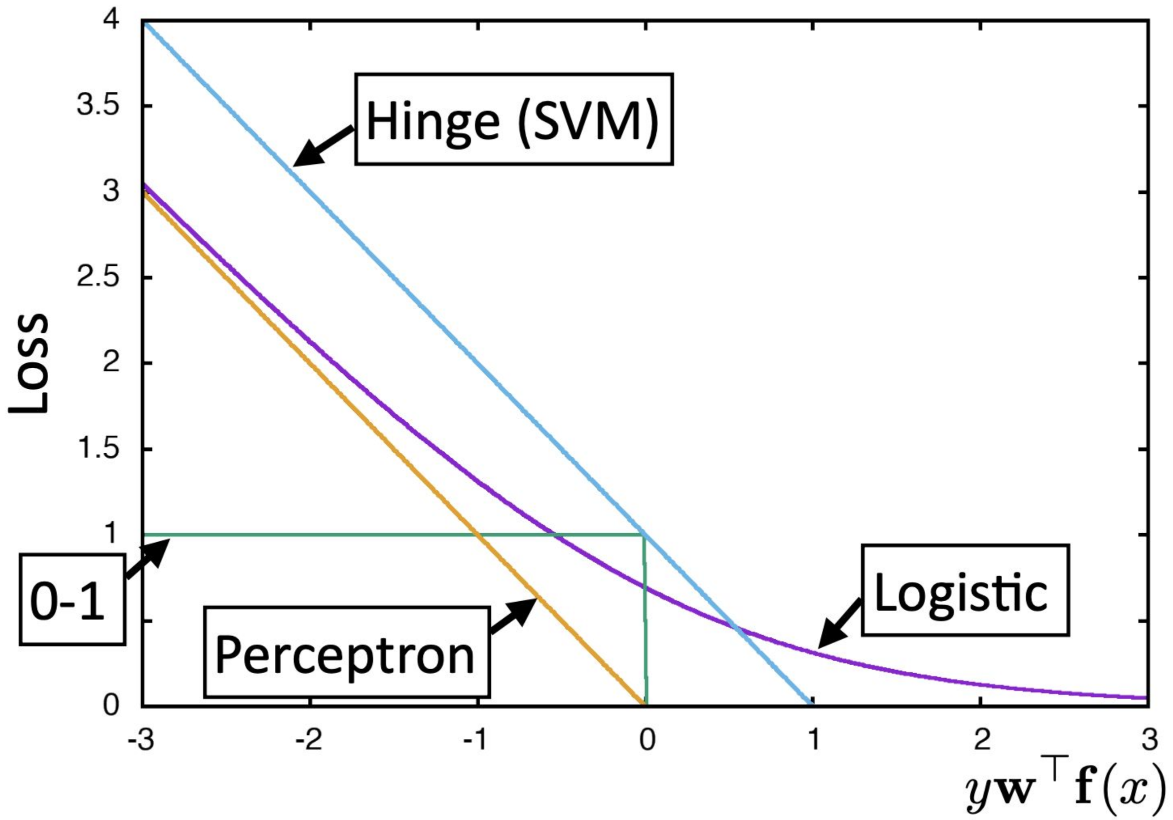
(Putting things in perspective)

$$\mathcal{L}_{\mathrm{lr}}(\mathbf{x}, y) = \begin{cases} -y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) + \log\left(1 + \exp\left(y\mathbf{w}^\top \mathbf{f}(\mathbf{x})\right)\right) & \text{if } y = +1 \text{ (positive)} \\ \log\left(1 + \exp\left(-y\mathbf{w}^\top \mathbf{f}(\mathbf{x})\right)\right) & \text{if } y = -1 \text{ (negative)} \end{cases}$$

$$\mathcal{L}_{\mathrm{perc}}(\mathbf{x}, y) = \begin{cases} 0 & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) > 0 \\ -y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) \leq 0 \end{cases}$$

Main differences:

- Perceptron: gradient-based optimization
- LR: probabilistic model
- Perceptron: if the data are linearly separable, perceptron is guaranteed to converge.
- LR: likelihood can never truly be maximized with a finite w vector.



Optimizers

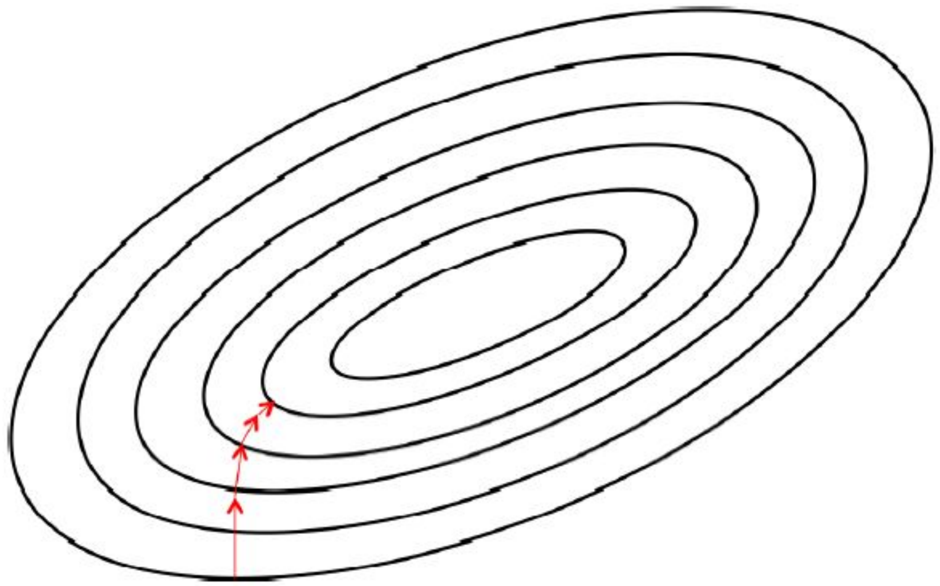
Gradient

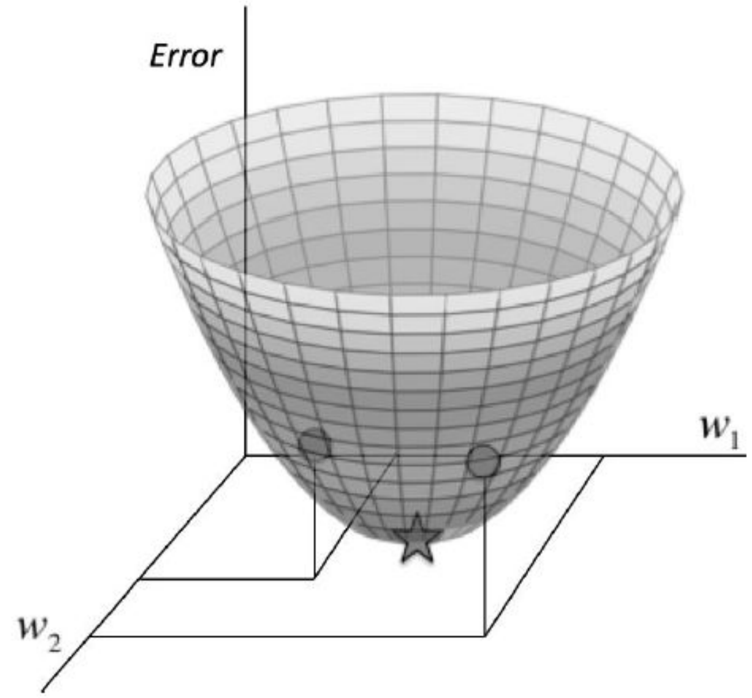
$$\Delta w_k = -\frac{\partial E}{\partial w_k}$$

$$= -\frac{\partial}{\partial w_k}\left(\frac{1}{m}\sum_i (w^T X_i - y_i)_i^2\right)$$

$$w_{i+1} = w_i + \Delta w_k$$

Stochastic gradient descent (**SGD**)





Optimizers

Practical test:
lr_val = [1; 0.1; 0.01]
momentum_val = 0
nesterov_val = ‘False'
decay_val = 1e-6

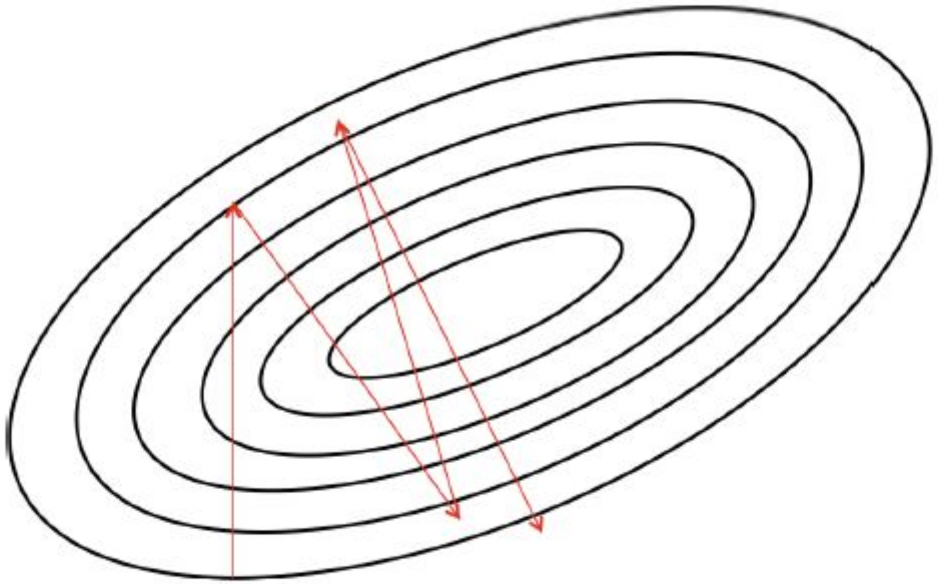
Hyperparameters

- Learning rate (α)

$$\Delta w_k = -\alpha \frac{\partial E}{\partial w_k}$$

$$= -\alpha \frac{\partial}{\partial w_k} \left(\frac{1}{m} \sum_i (w^T X_i - y_i)_i^2 \right)$$

$$w_{i+1} = w_i + \Delta w_k$$

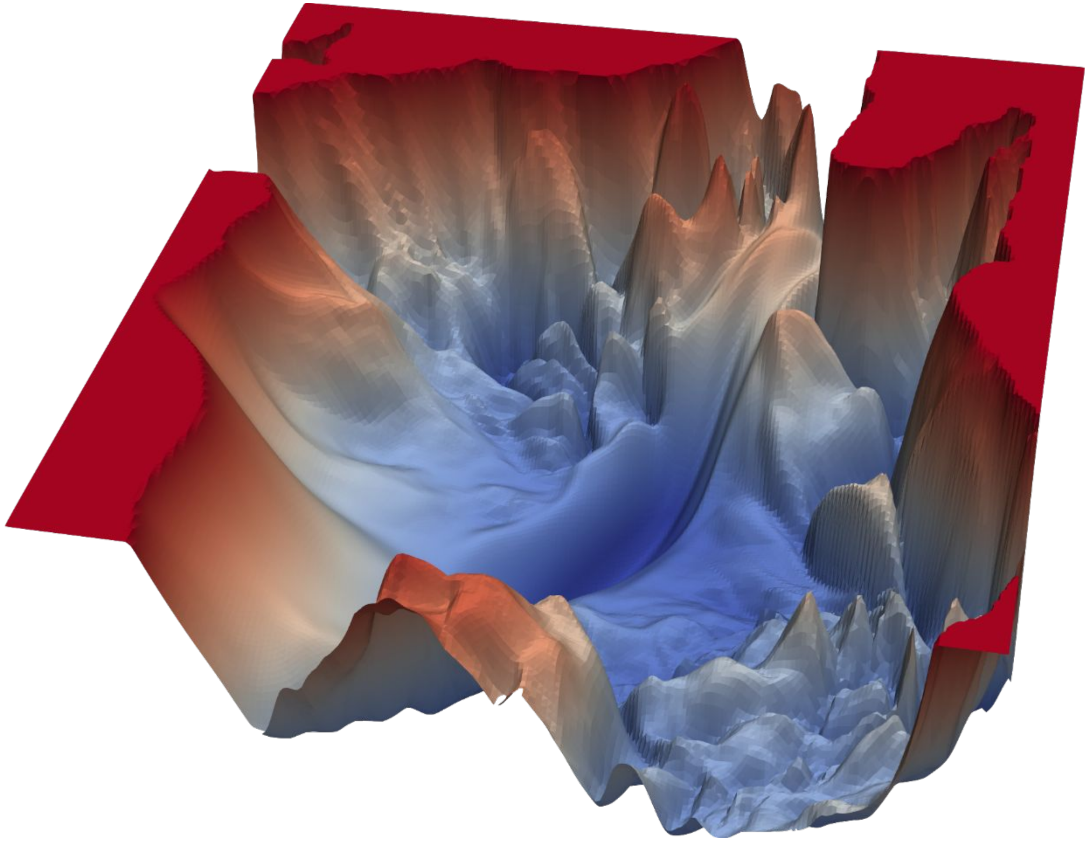


Result of a large learning rate α

Stochastic gradient descent (**SGD**)

Optimizers

Watch out for local minimal areas



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