SPATIAL ECOLOGY

# Perceptron

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# Agenda

1) Finalize SVM/SVR (remaining from Class 1)

2) Introduction to optimization

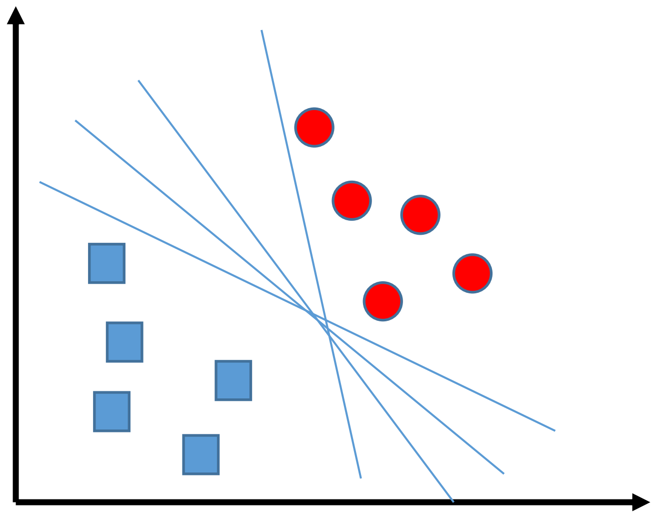
- Review on Linear Regression
- Minimizing loss functions
- Regularization

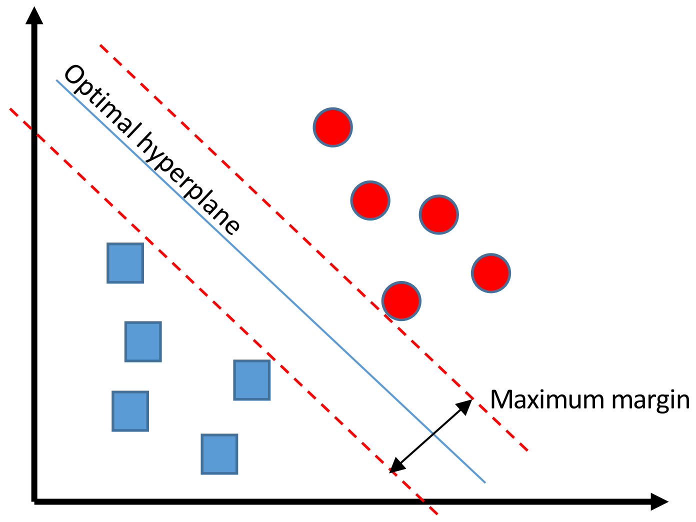
3) Perceptron

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

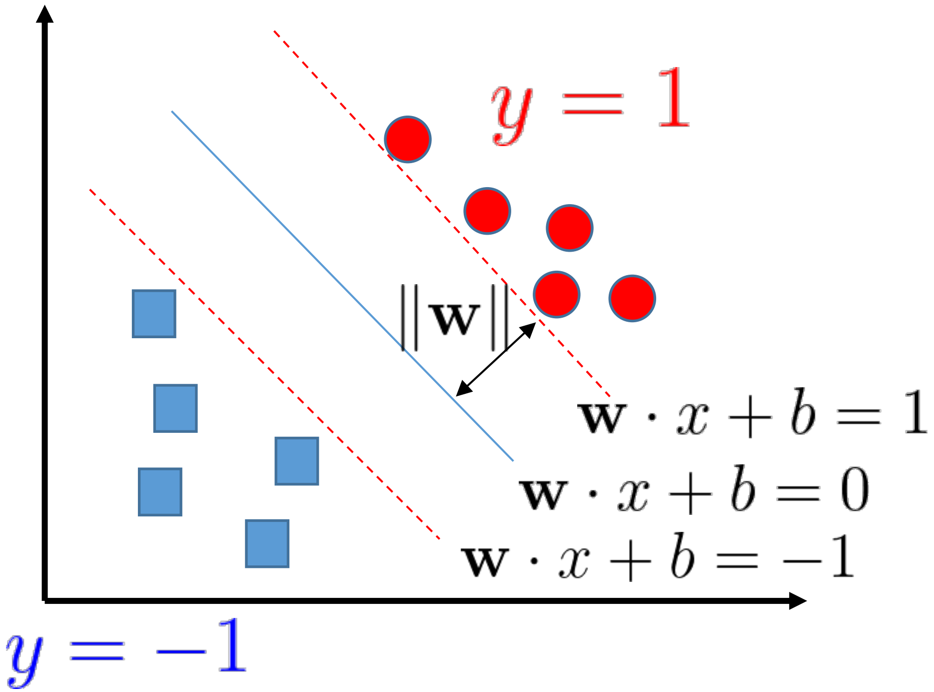
# Support Vector Machine

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





# Support Vector Machine




Hyperplane equation: $f(x) = \mathbf{w} \cdot x + b$

Distance (D) from a point to the hyperplane

$$D = \frac{|\mathbf{w} \cdot x + b|}{\|\mathbf{w}\|}$$

Minimize the weights, increase distance

Classification task

$$\begin{cases} wx_i + b \geq +1 & \text{when } y_i = +1 \\ wx_i + b \leq -1 & \text{when } y_i = -1, \end{cases}$$

# 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

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

Updating the weights:

No misclassification

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

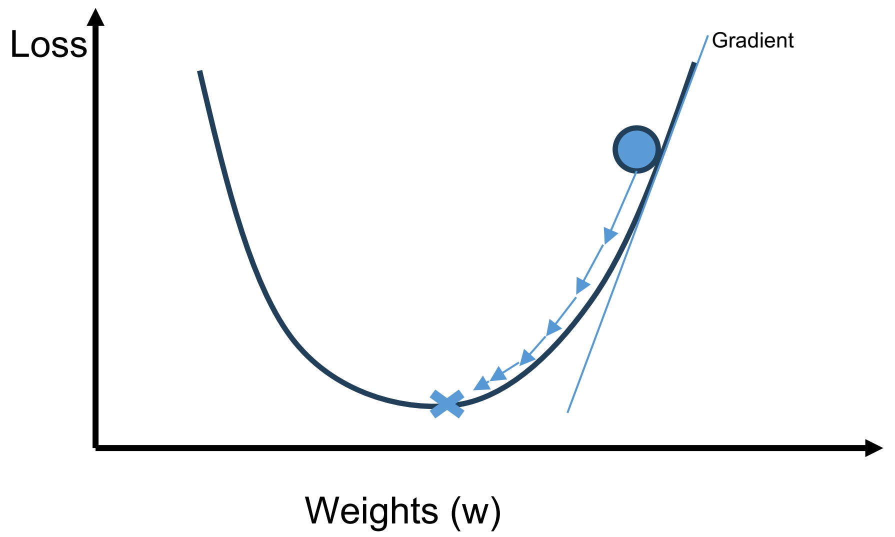
Misclassification

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

Gradients

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

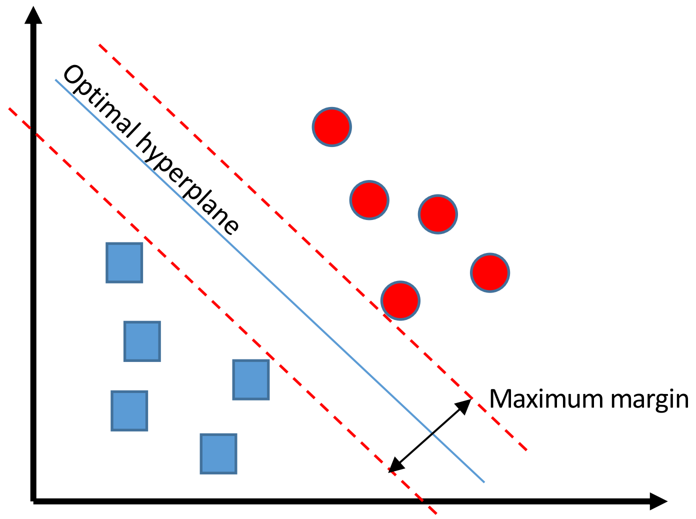
$$\frac{\delta}{\delta w_k} \big(1 - y_i \langle x_i, w \rangle\big)_+ \quad = \begin{cases} 0, & \text{if } y_i \langle x_i, w \rangle \geq 1 \\ -y_i x_{ik}, & \text{else} \end{cases}$$



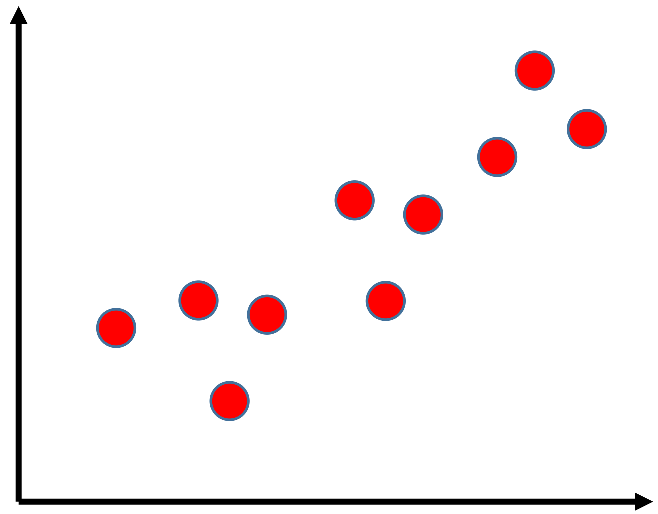
# Support Vector Machine for Regression

How do I turn the SVM into a SVR?

SVM




SVR(?)



# SVR Optimization

Loss

$$L(y, f(x, \mathbf{w})) = \begin{cases} 0, & |y - f(x, \mathbf{w})| \le \epsilon \\ |y - f(x, \mathbf{w})| & \text{o.w.} \end{cases},$$

Constraints

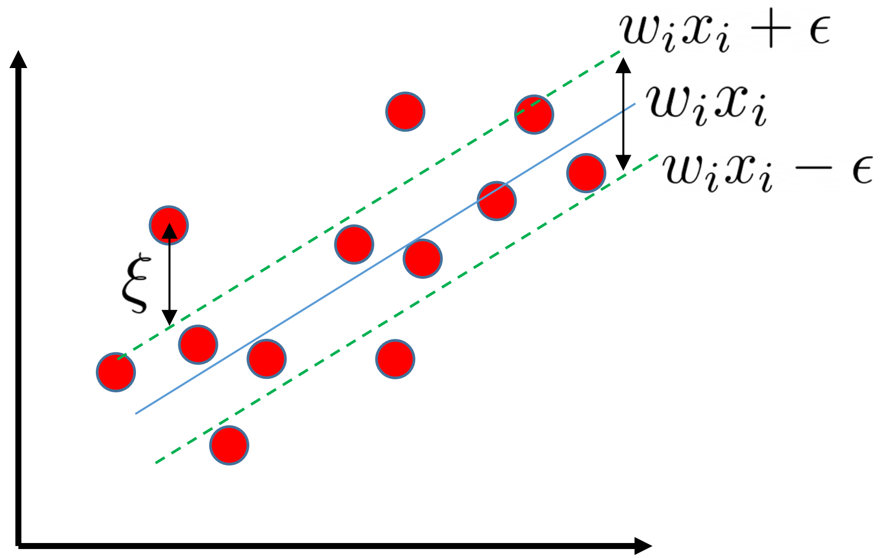
$$|y_i - w_i x_i| \le \epsilon + |\xi_i|$$

Deviation from the margin (slack)

Margin of error

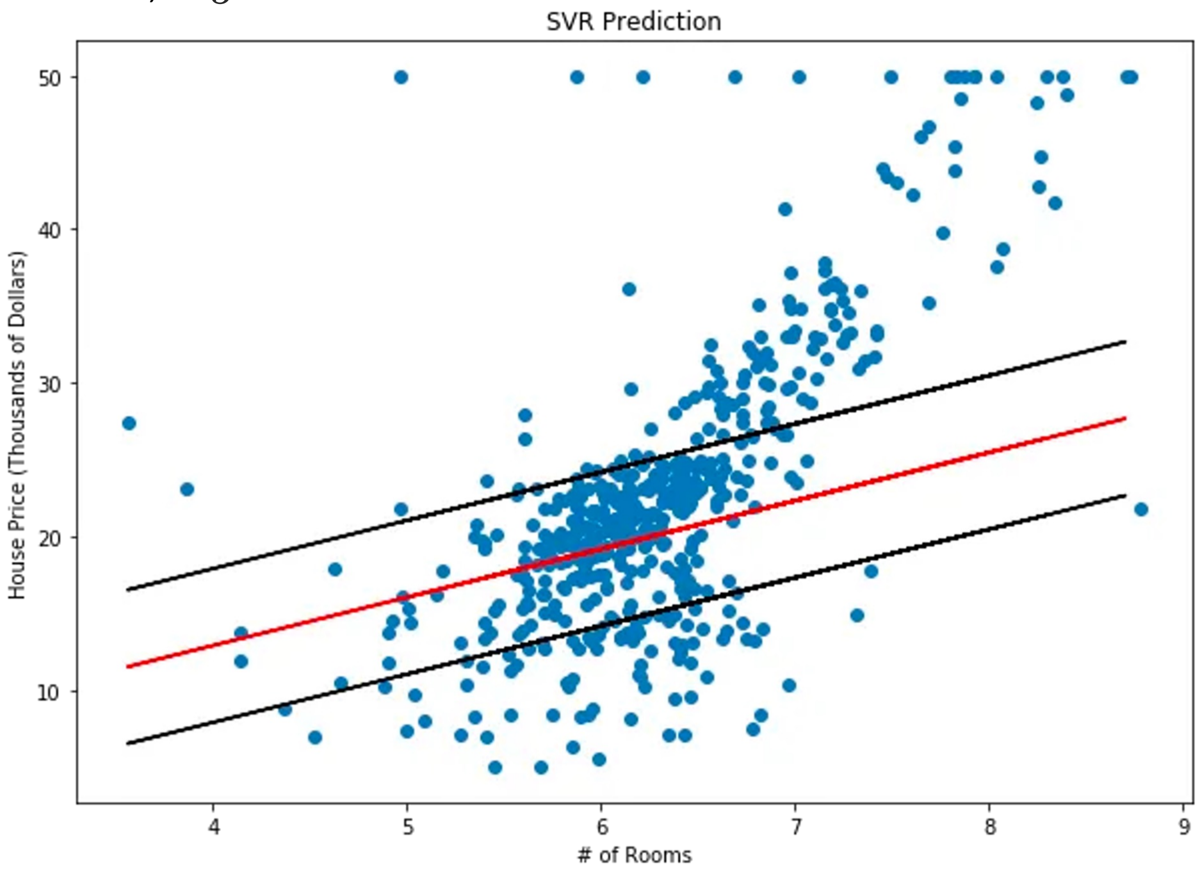
Loss function for the SVR

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



# Example: House price in Boston

SVR, $\epsilon$=5

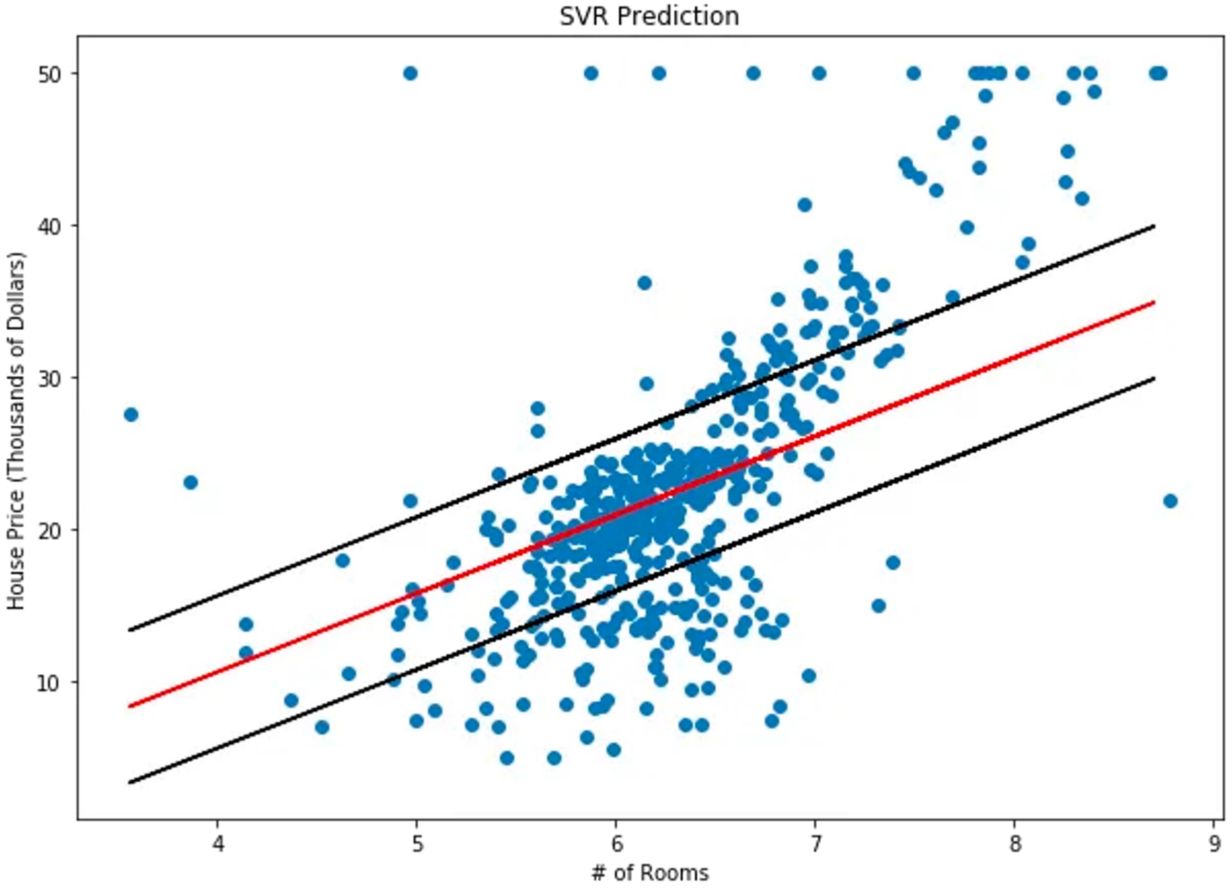



Conclusions:

- Several the points still fall outside the margins
- Consider the possibility of errors that are larger than ϵ
- Add some slack

# Example: House price in Boston

SVR, $\epsilon$=5, $C$=1.0

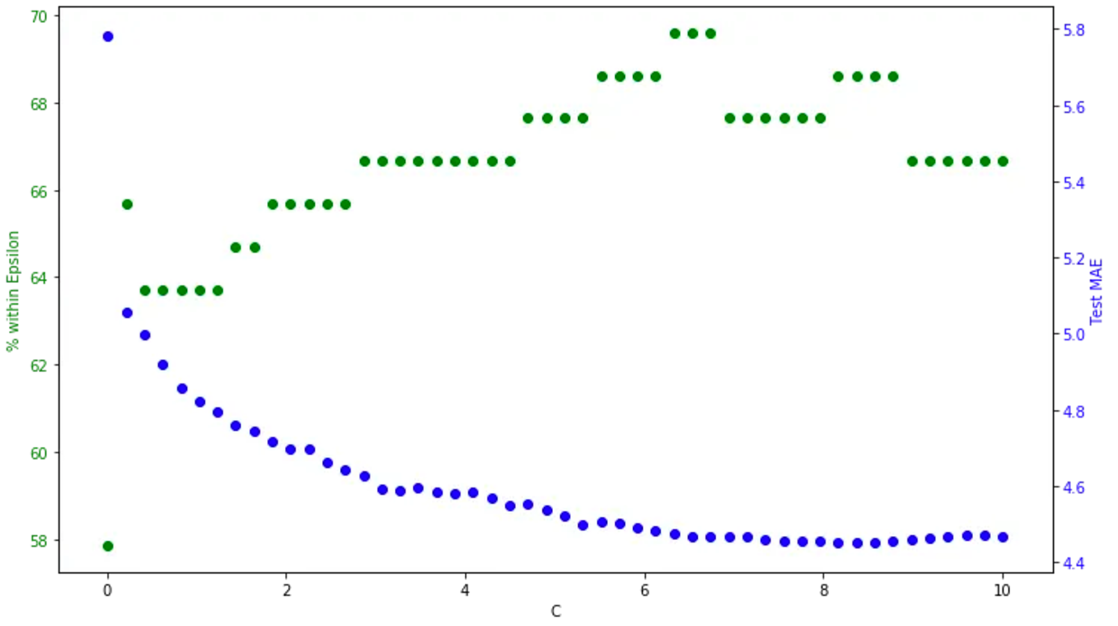



Conclusions:

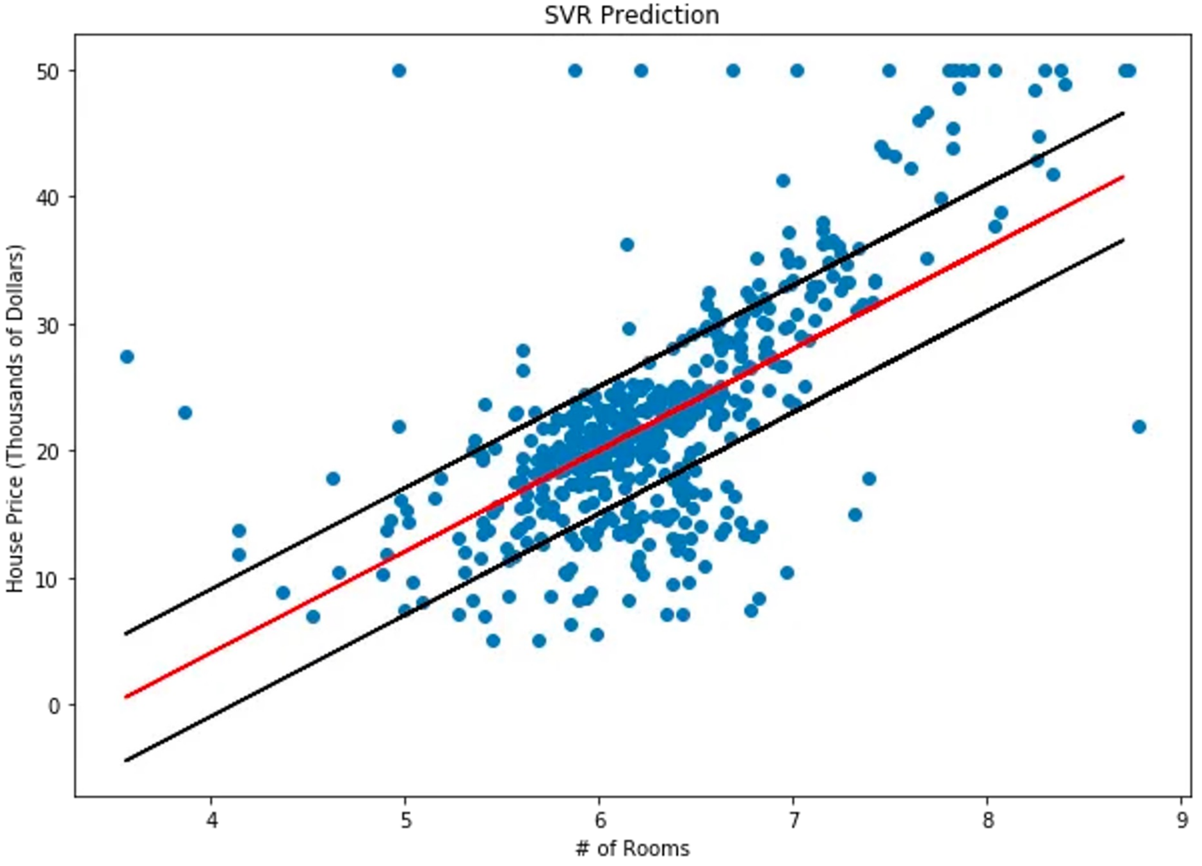
- As $C$ increases, our tolerance for points outside of $\epsilon$ also increases.
- As $C$ approaches 0, the tolerance approaches 0 and the equation collapses into the simplified (although sometimes infeasible) one.

# Example: House price in Boston

- We can use grid search over *C* to find the ideal amount of slack (more points within margin).
- Since our original objective of this model was to maximize the prediction within our margin of error ($5,000), we want to find the value of *C* that maximizes *% within Epsilon*. Thus, *C*=6.13.




$\epsilon$=5, $C$=6.13



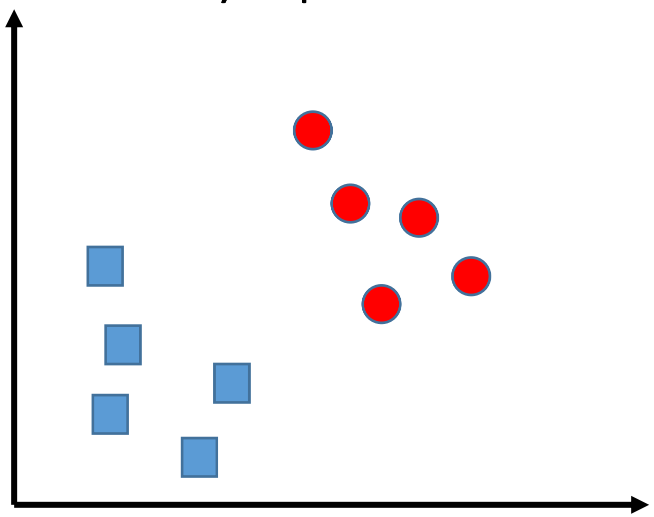
# Support Vector Machine for Regression

- 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.

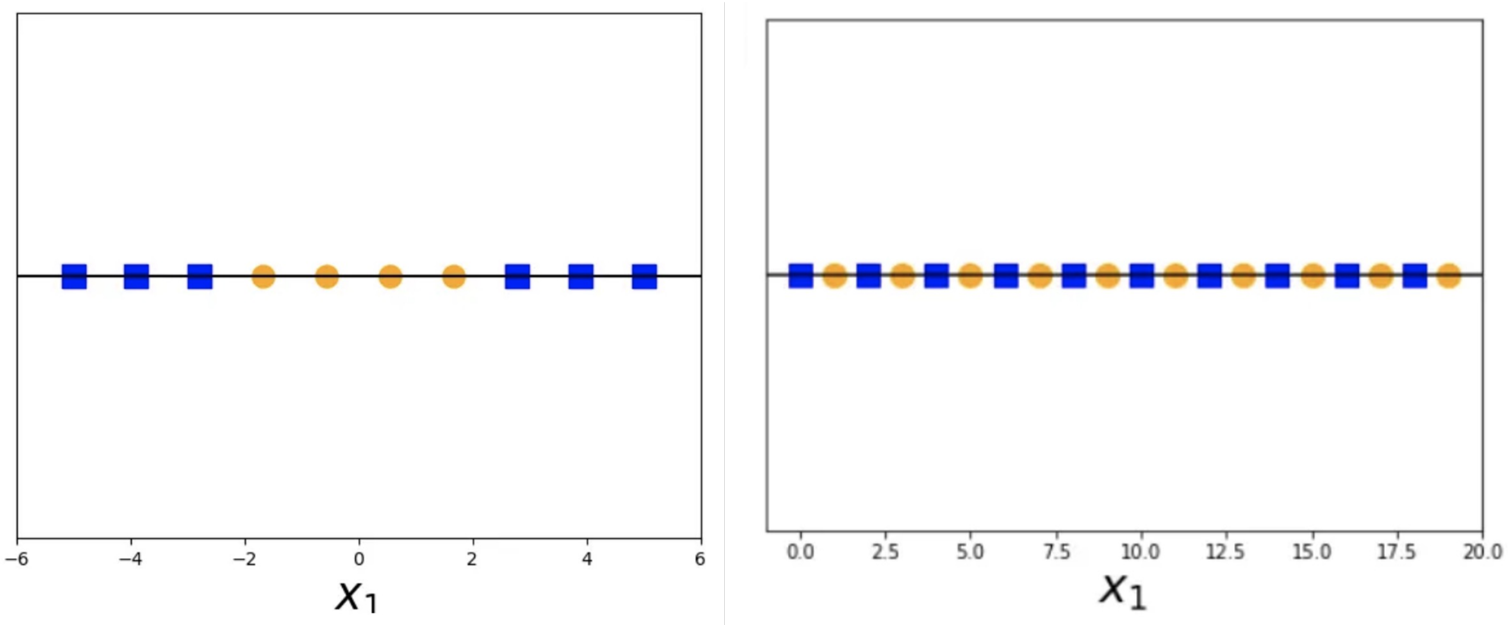
# What if…

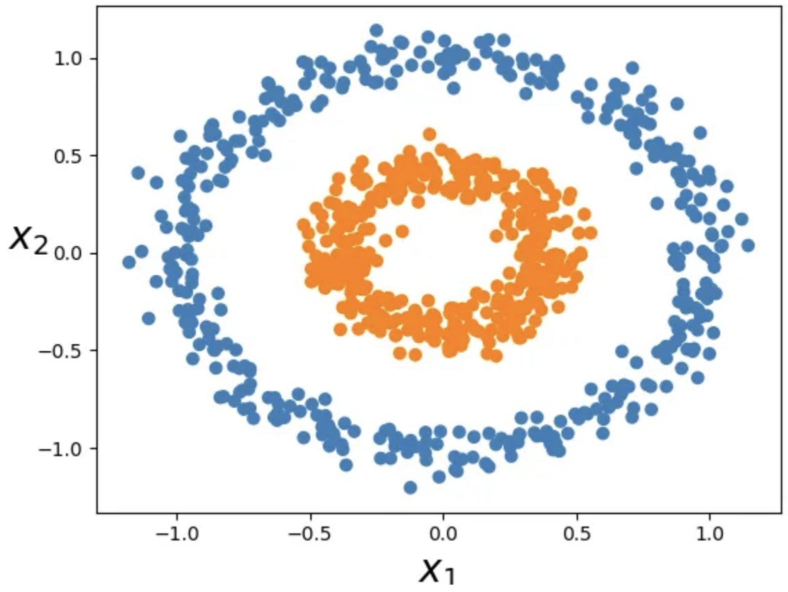
## Non-linear spaces

Linearly separable

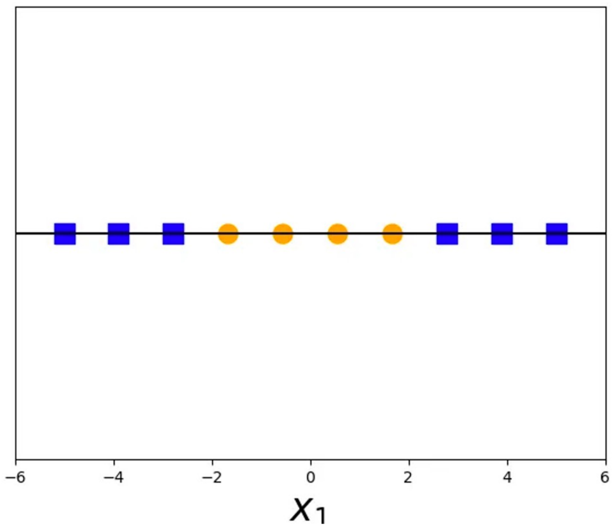


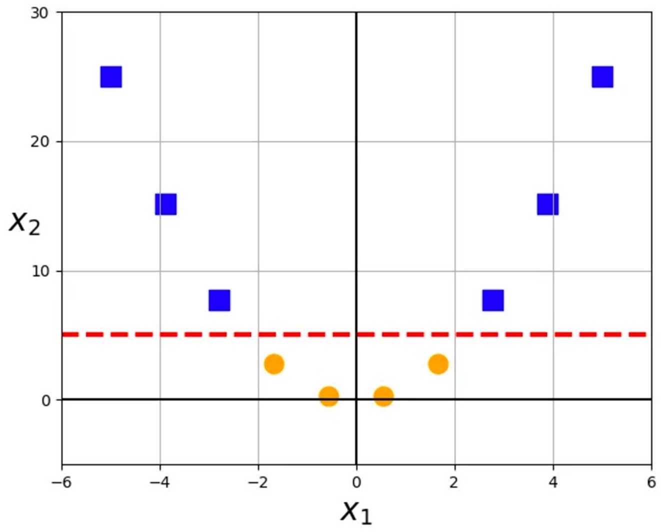
Not linearly separable



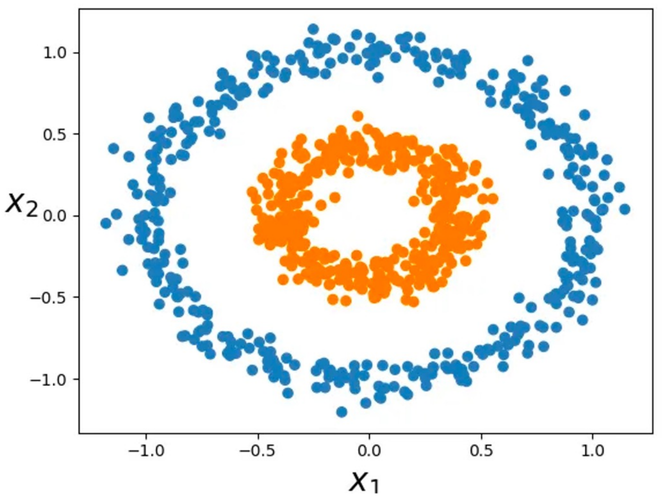
# Kernel tricks

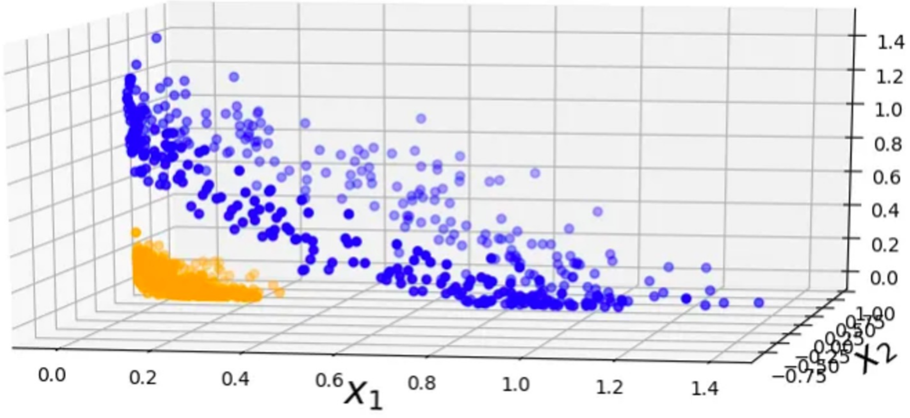



*"Give me enough dimensions and I will classify the whole world".*

*Zucker, Steve*



# Time for a quiz and tutorial!

https://tinyurl.com/GeoComp2024

# Intro to optimization

# 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)*

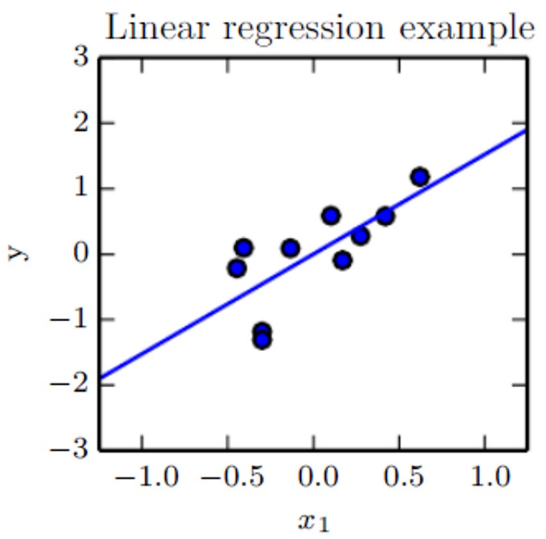
$$MSE_{test} = \frac{1}{m} \sum_i (\hat{y}_{test} - y_{test})_i^2$$

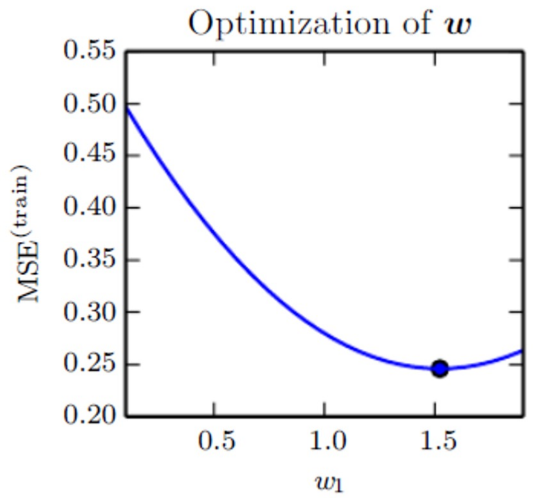
*Dataset*

$$(X, y) \quad \begin{cases} (X_{train}, y_{train}) \\ (X_{test}, y_{test}) \end{cases}$$

*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)

# Linear Regression Optimization

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

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

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

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

# Mean squared error loss

Rewrite:

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

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

# Regularization

- Ridge regression: penalize with L2 norm

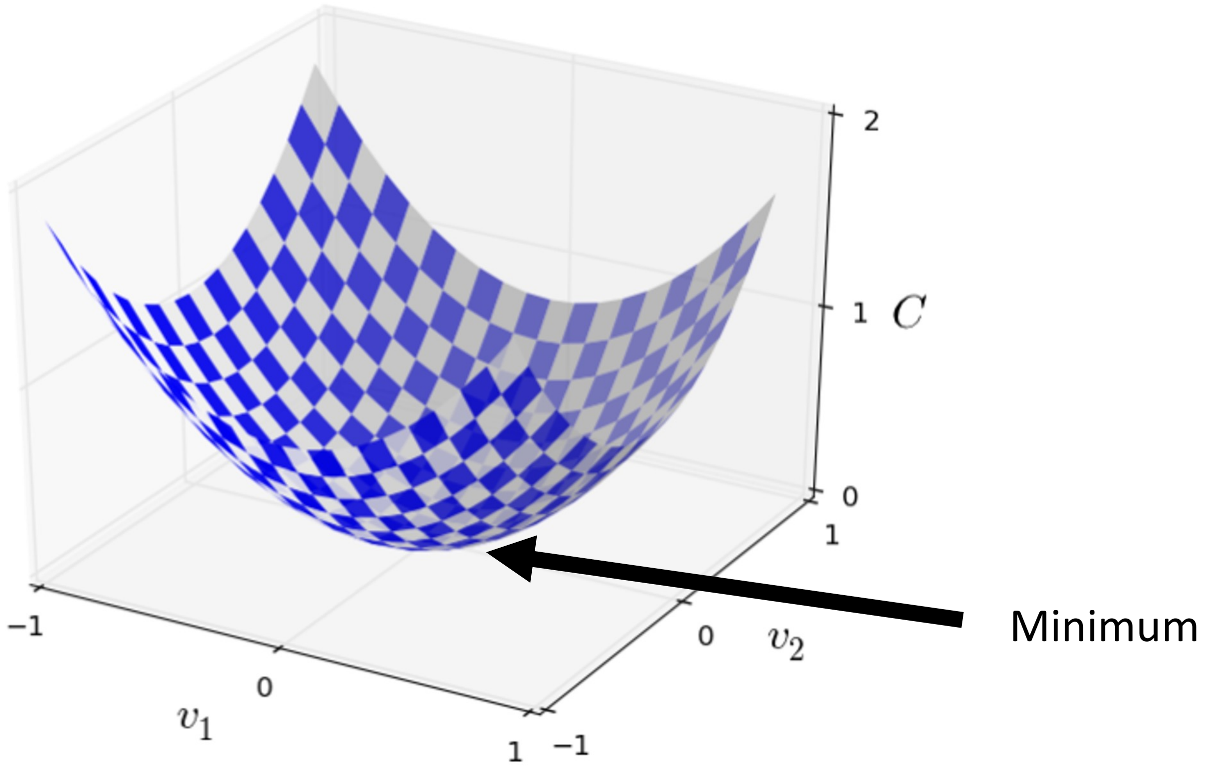
$$\boldsymbol{w}^* = \arg\min \sum_i L(f(\boldsymbol{x}_i; \boldsymbol{w}), y_i) + \lambda \sum_{j=1}^{m} w_j^2$$

  - Closed form solution exists $\boldsymbol{w}^* = (\lambda I + X^T X)^{-1} X^T \boldsymbol{y}$
- LASSO regression: penalize with L1 norm

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

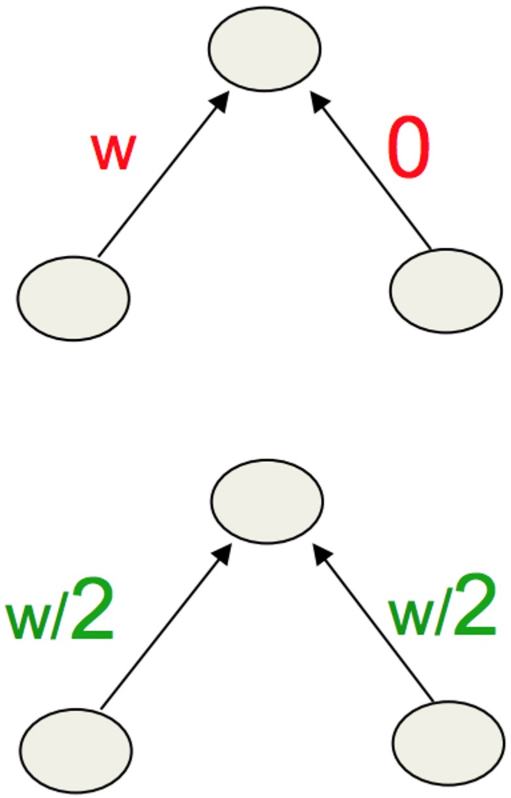
  - No closed form solution but still convex (optimal solution can be found)

# 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!

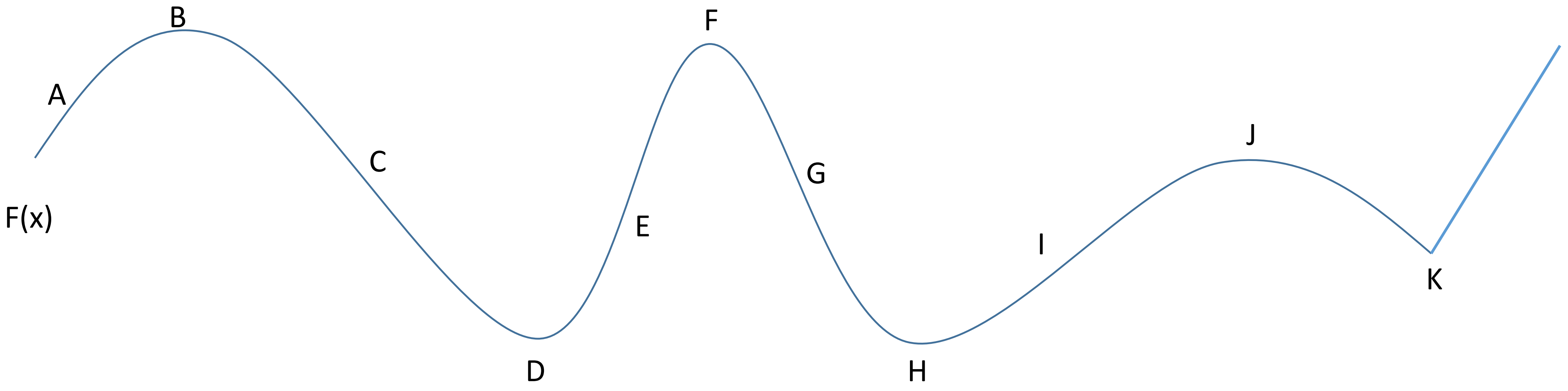
# Regularization



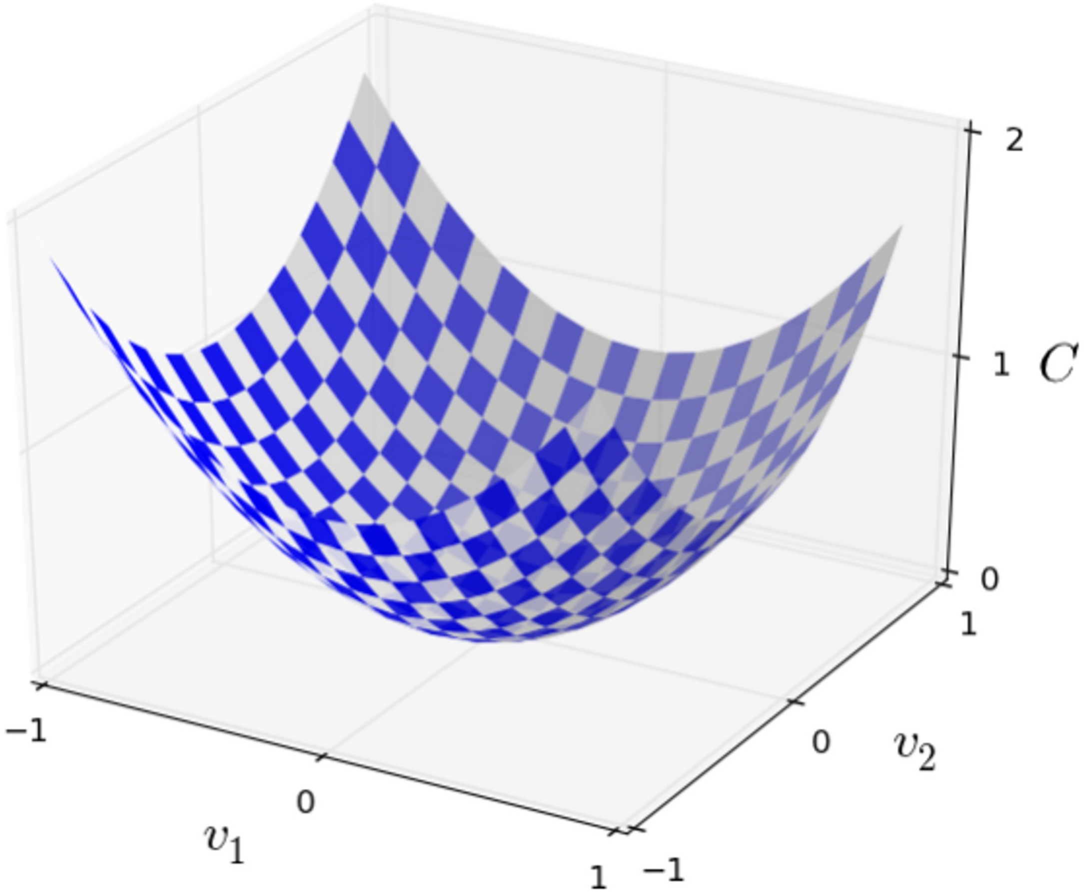

- Prefers to share smaller weights
- Makes model smoother
- More Convex

# More on the derivatives

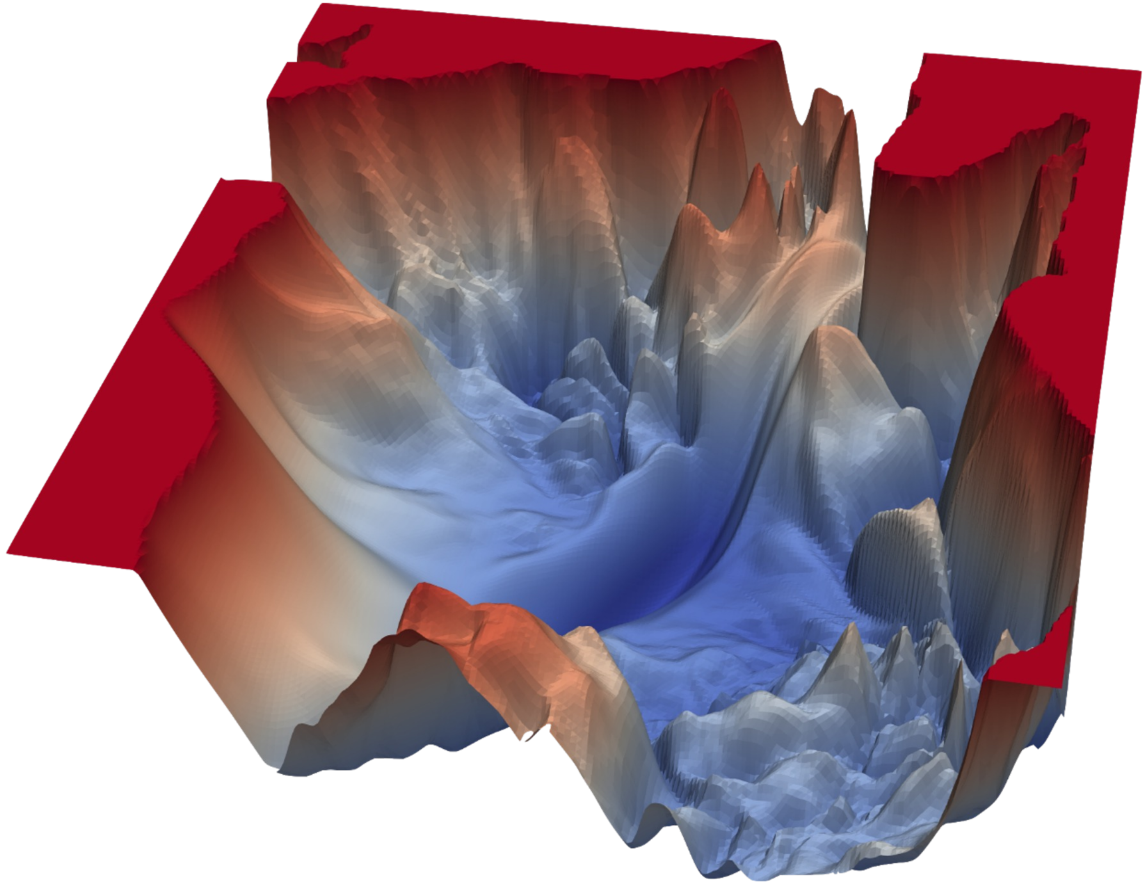
https://tinyurl.com/GeoComp2024



Expectation

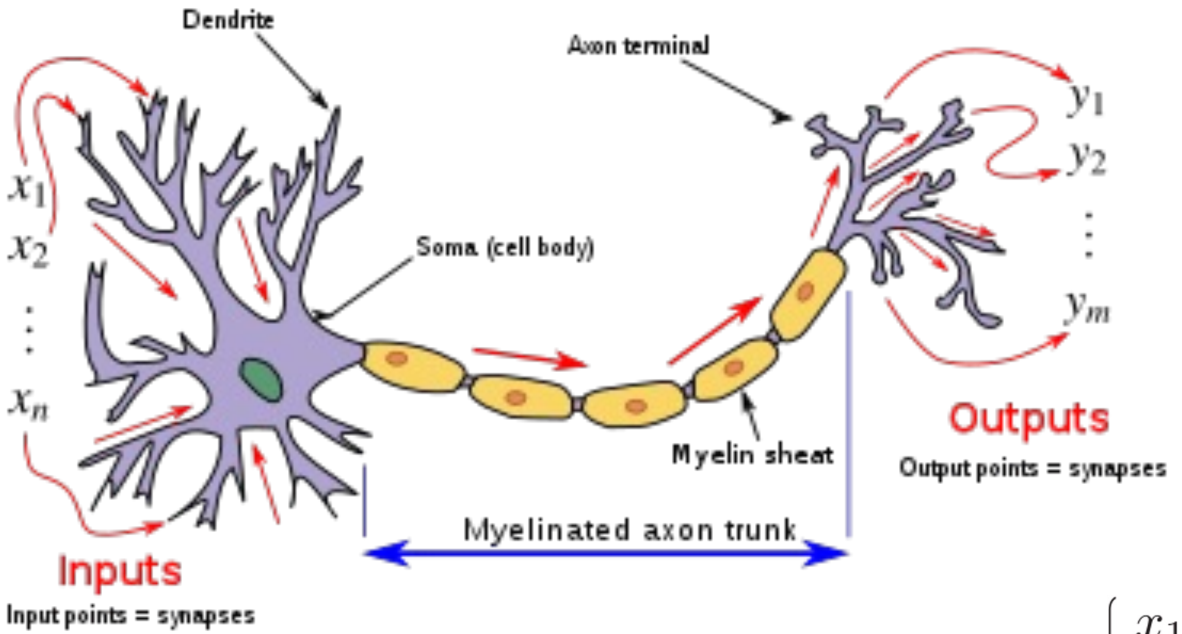


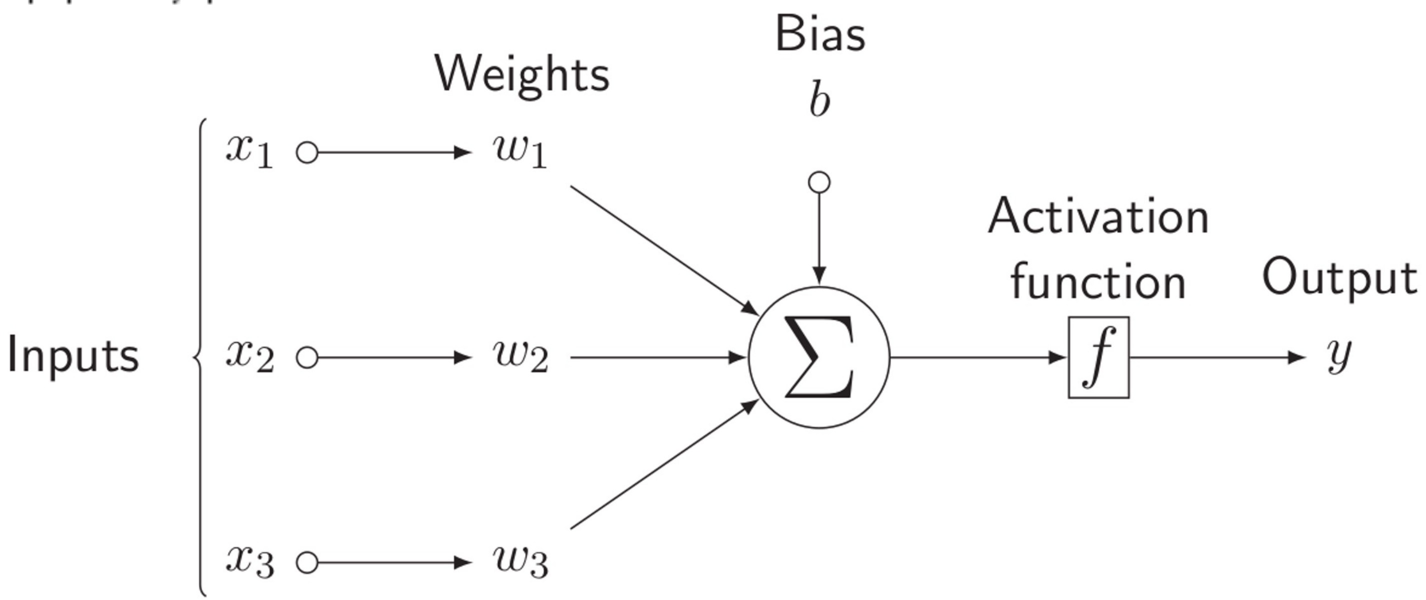

Reality



# Perceptron

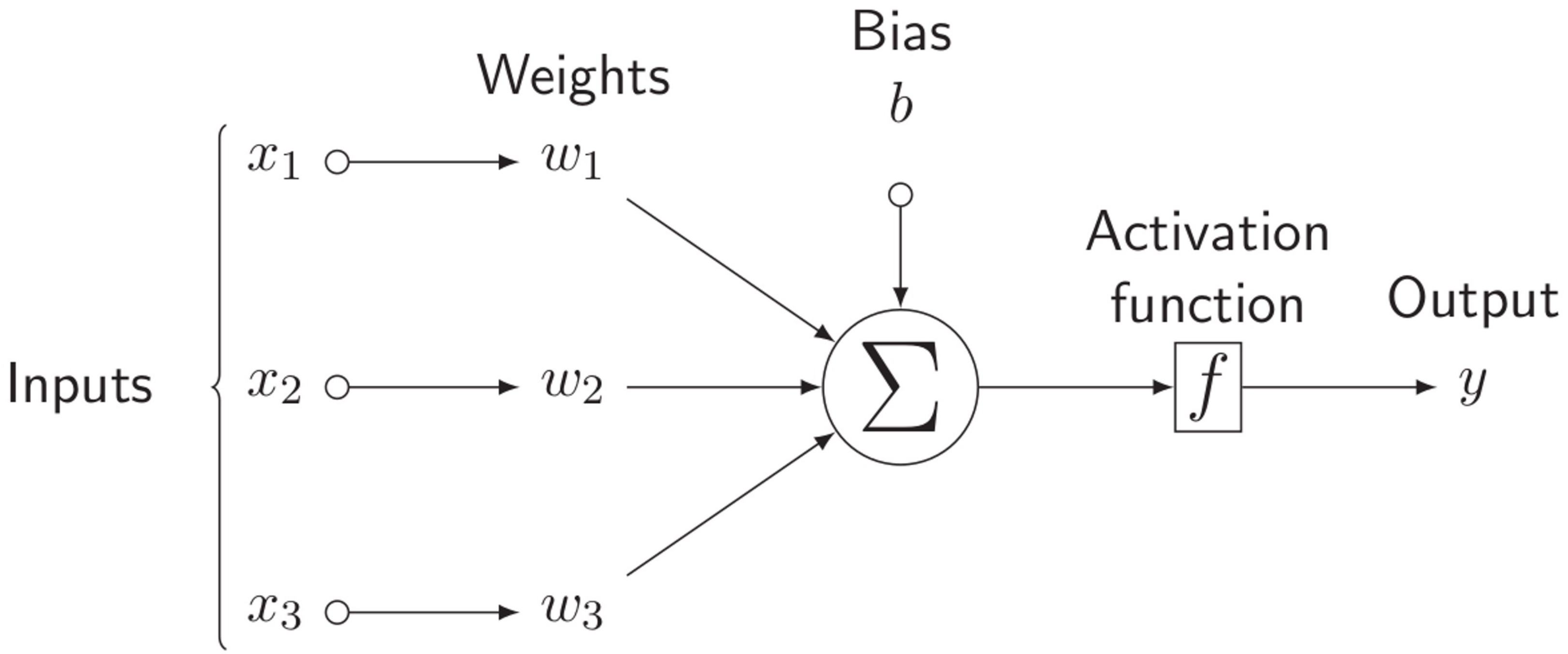
# Perceptron: Threshold Logic



# Perceptron: Threshold Logic

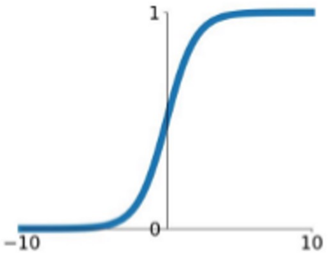
$$\mathcal{L}_{\text{perc}}(\mathbf{x}, y) = \begin{cases} 0 & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) > 0 \\ -y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) \leq 0 \end{cases}$$



# Activation functions

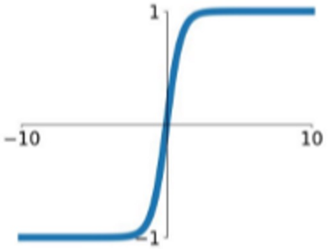
**Sigmoid**

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



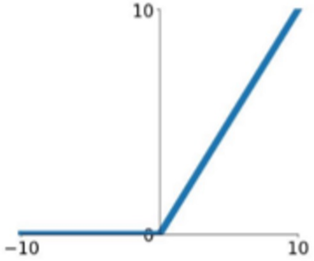

**tanh**

$\tanh(x)$



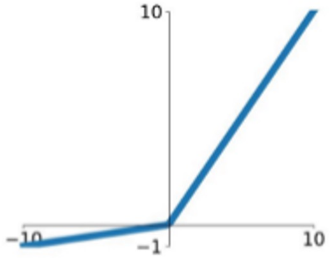

**ReLU**

$\max(0, x)$




**Leaky ReLU**

$\max(0.1x, x)$

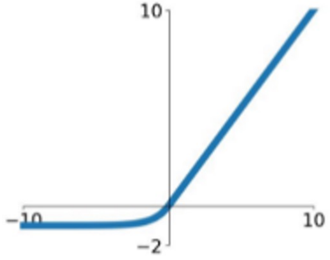



**Maxout**

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

**ELU**

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



# Optimizers

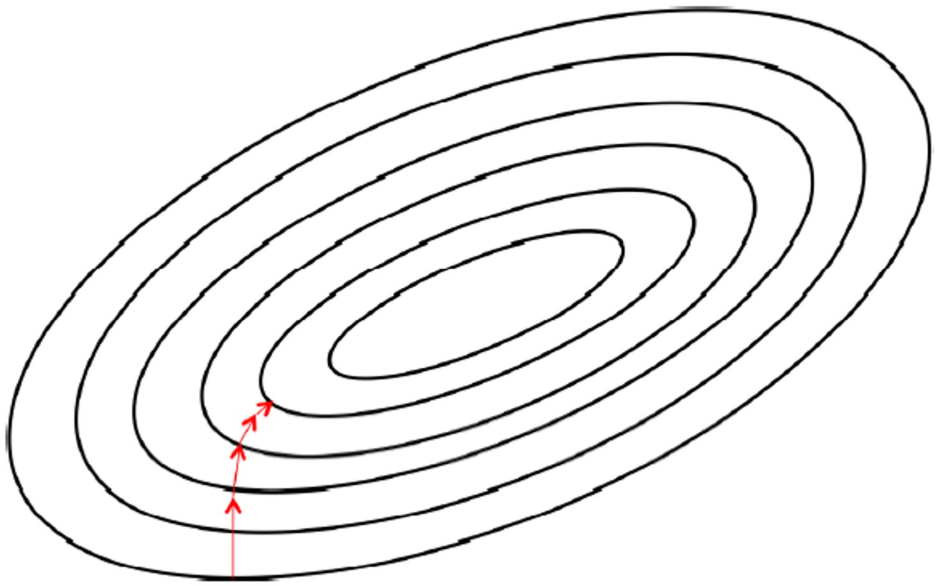
Gradient

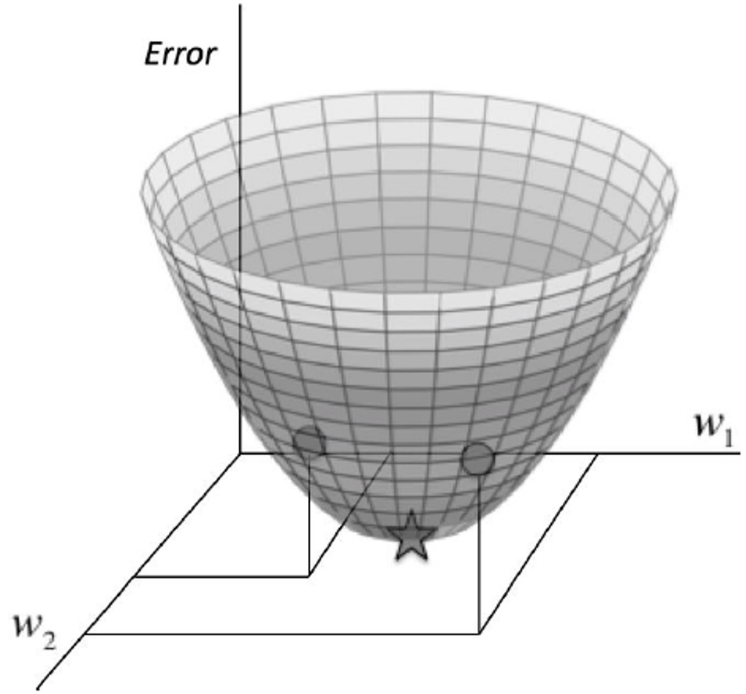
$$\Delta w_k = -\frac{\partial E}{\partial w_k}$$

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

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

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

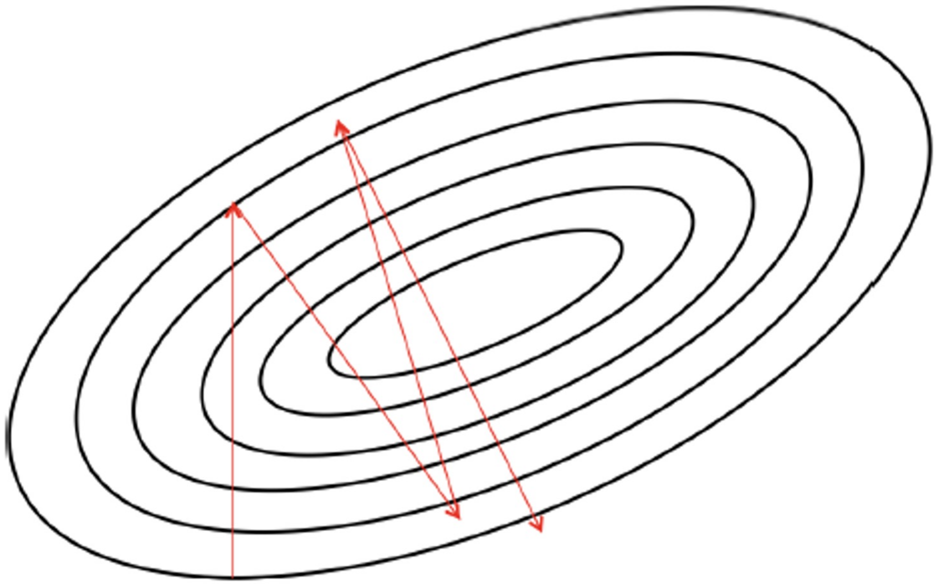
- Learning rate ($\alpha$)

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

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

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

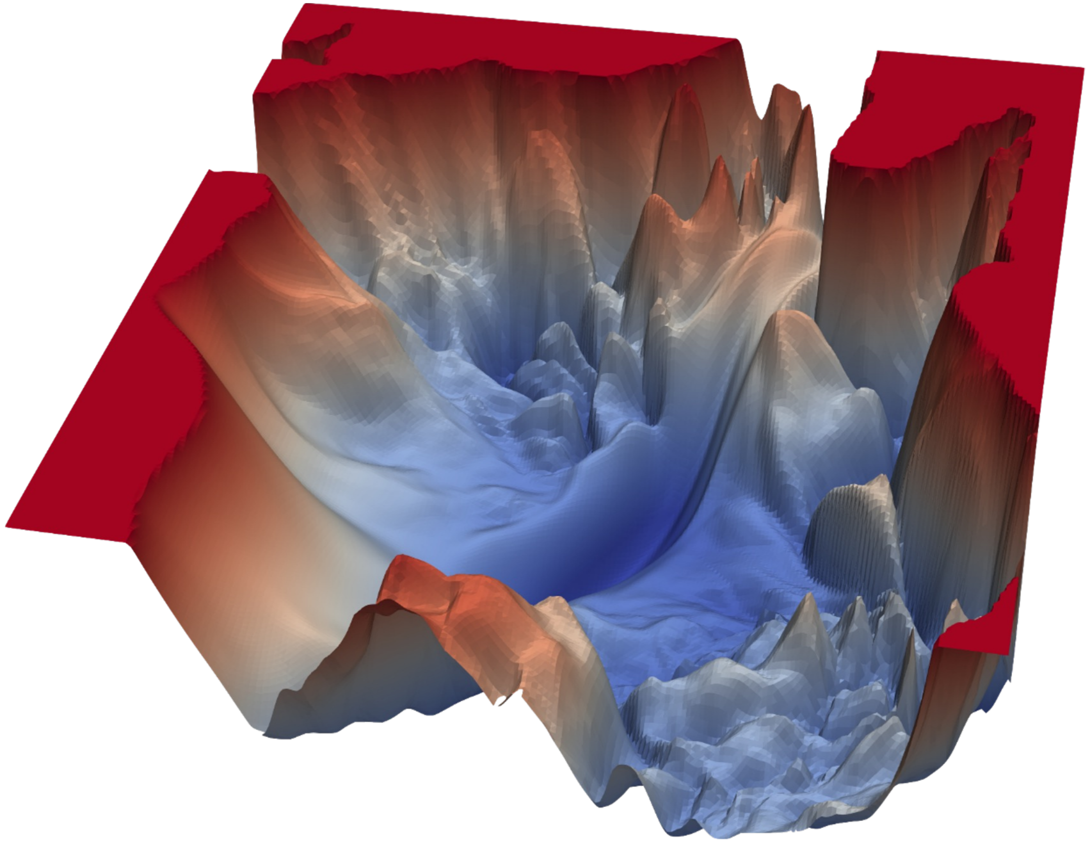
Stochastic gradient descent (**SGD**)



Result of a large learning rate $\alpha$

# Optimizers

Watch out for local minimal areas



Hyperparameters

- Learning rate ($\alpha$)

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

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

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

Stochastic gradient descent (**SGD**)

# Gradient Descent

- Gradient descent refers to taking a step in the direction of the ***gradient (partial derivative)*** of a weight or bias with respect to the loss function
- Gradients are propagated backwards through the network in a process known as ***backpropagation***
- The size of the step taken in the direction of the gradient is called the ***learning rate***

# Time for a quiz and tutorial!

https://tinyurl.com/GeoComp2024