COMP0169: Machine Learning for Visual Computing

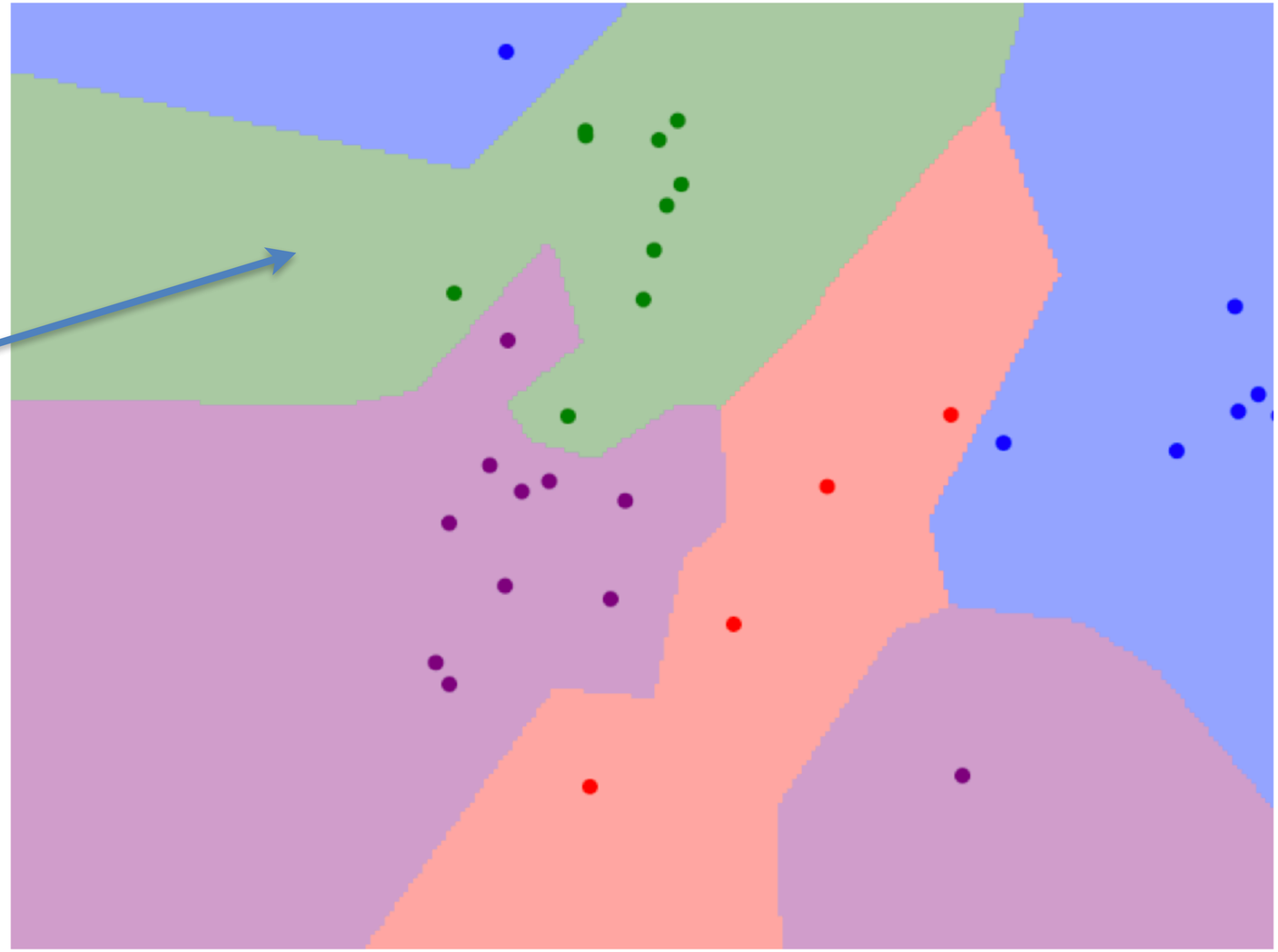
PCA and Linear Classifiers

Lectures will be Recorded

Recap

- Different ML tasks in VC
- Nearest neighbors and kNN classifier
- XOR problem

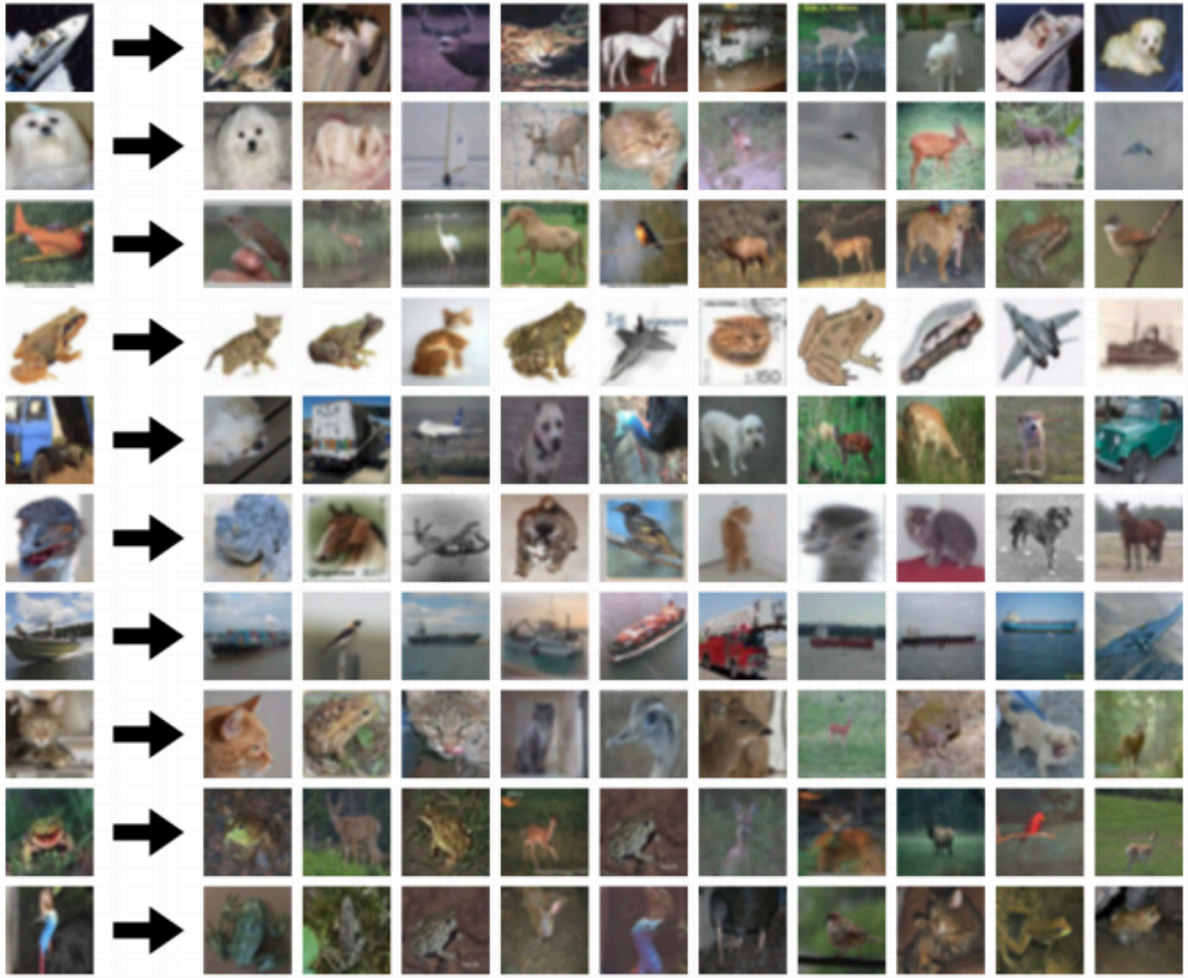
Nearest Neighbor Explained



I_x

- Decision boundary
- Jagged boundary
- Isolated regions
- Error prone
- Training time O(1)
- Test time O(n)

How Does It Perform?

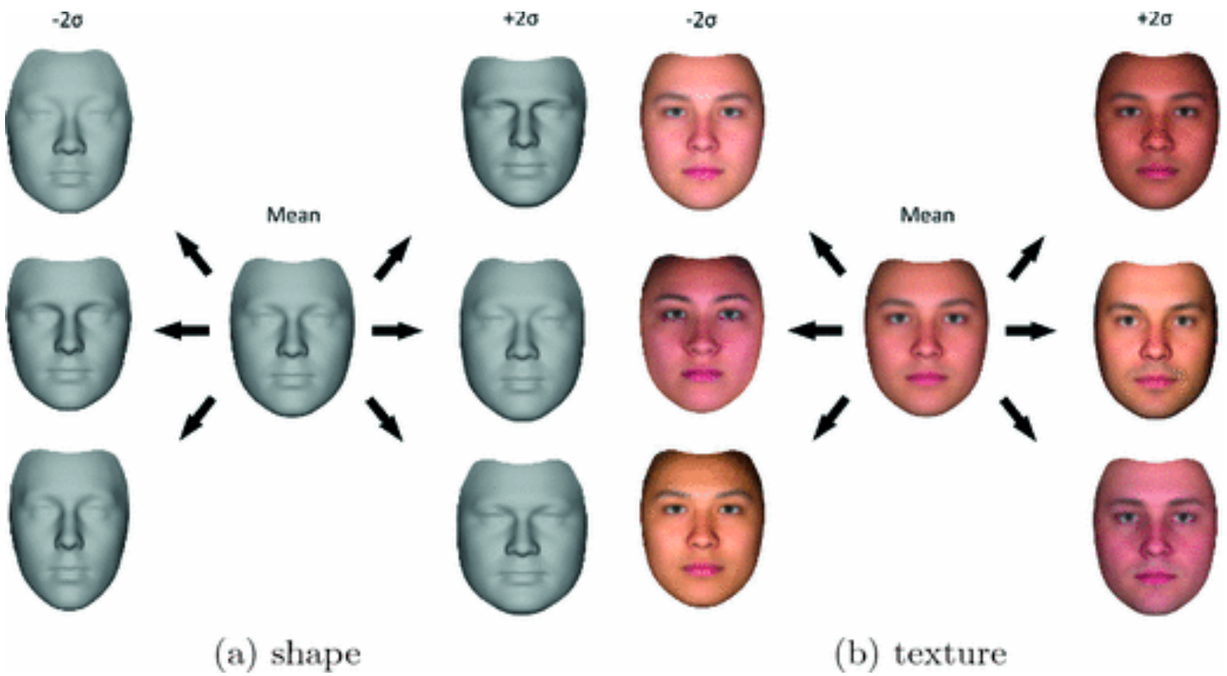


Principal Component Analysis

- **Problem setup** $\{\mathbf{x}_1, \ldots \mathbf{x}_n\}$ **with** $\mathbf{x}_i \in \mathbb{R}^p$
- **(Optional) Scale variables to unit length**
- **Mean centering** $\mathbf{x}_i \leftarrow \mathbf{x}_i - \bar{\mathbf{x}}$
- **Covariance matrix** $C = X^T X$
- **Eigen analysis** $C = Q \Lambda Q^T$
- **Or, SVD** $X = U \Sigma W^T$

$$C = X^T X = W \Sigma^2 W^T$$

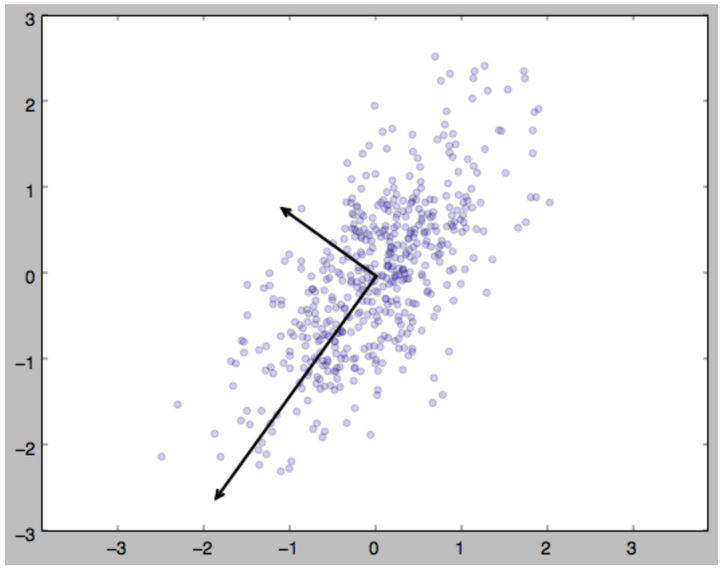
Morphable Faces



Video at http://gravis.dmi.unibas.ch/Sigg99.html

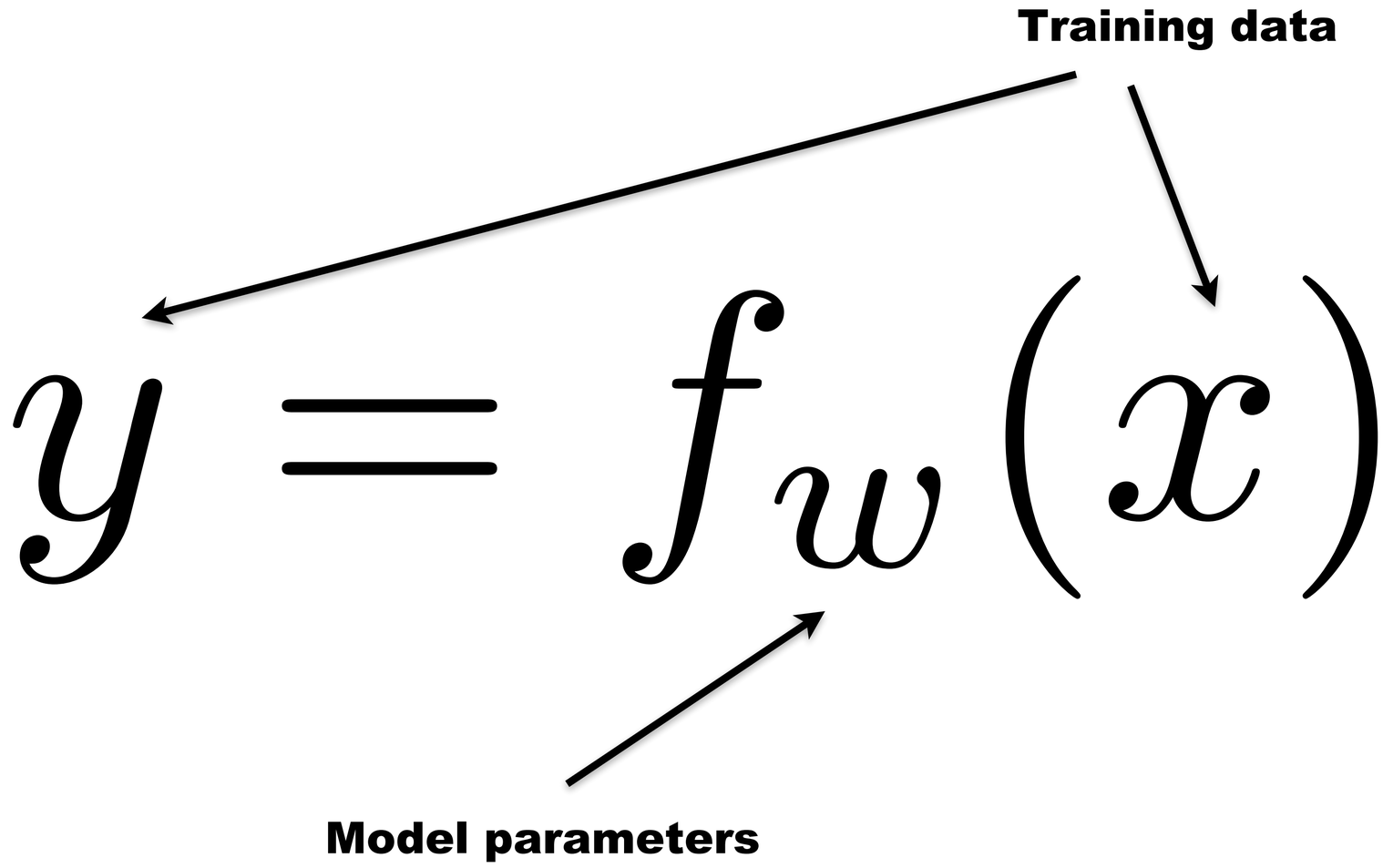
Wood et al., 2021 Arxiv,
Fake it till you make it: face analysis in the wild using synthetic data alone

Code Example

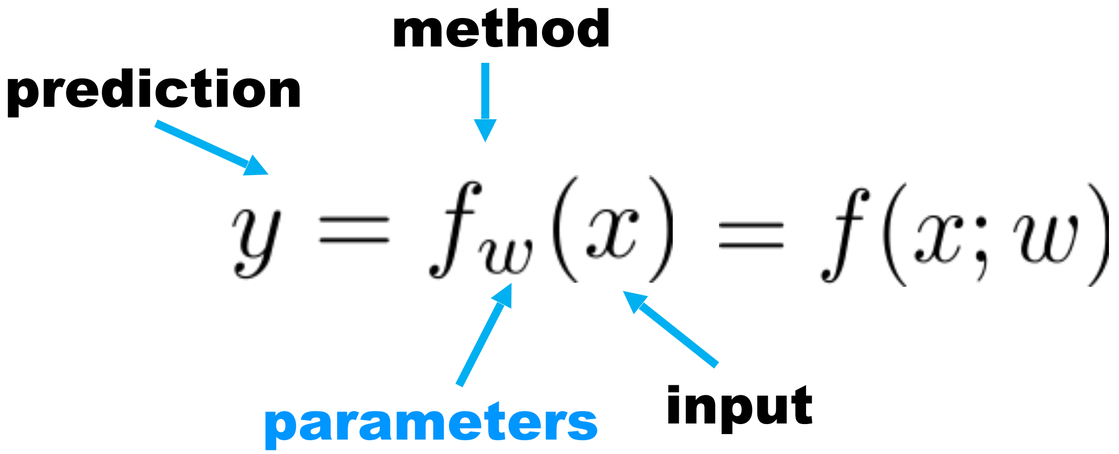


```
mean_vec = np.mean(X, axis=0)
cov_mat = (X - mean_vec).T.dot((X - mean_vec)) / (X.shape[0]-1)
matU, sigma, matV = np.linalg.svd(cov_mat)
```

Learning a Function



Learning a Function: Modeling

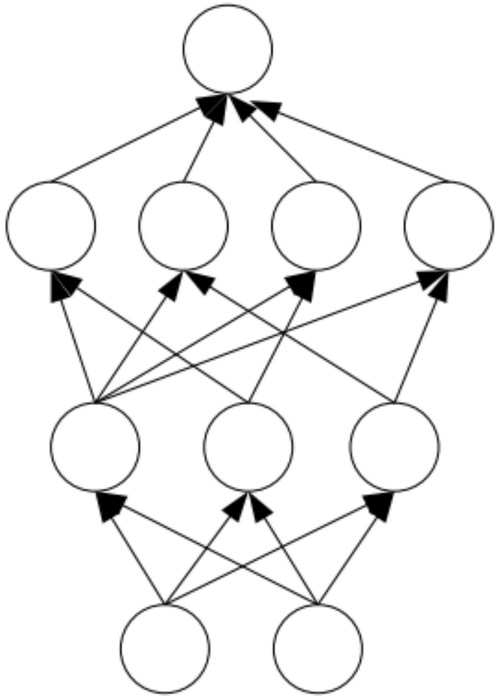


$$w \in \mathbb{R}$$

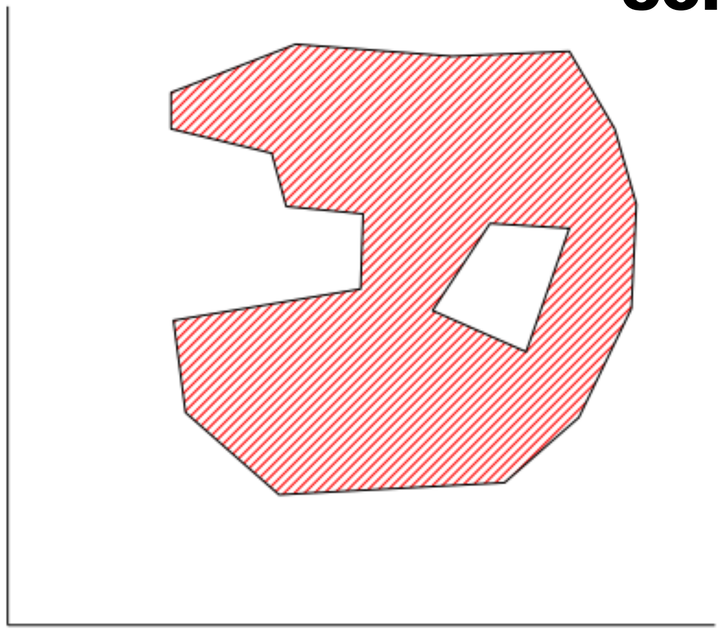
$$\mathbf{w} \in \mathbb{R}^K$$

Combining Simple Functions/Classifiers

3 layers of trainable weights



complex polygons



composition of polygons: convex regions

Regression

1. Least Squares fitting

2. Nonlinear error function and gradient descent

3. Perceptron training

Regression

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2. Nonlinear error function and gradient descent

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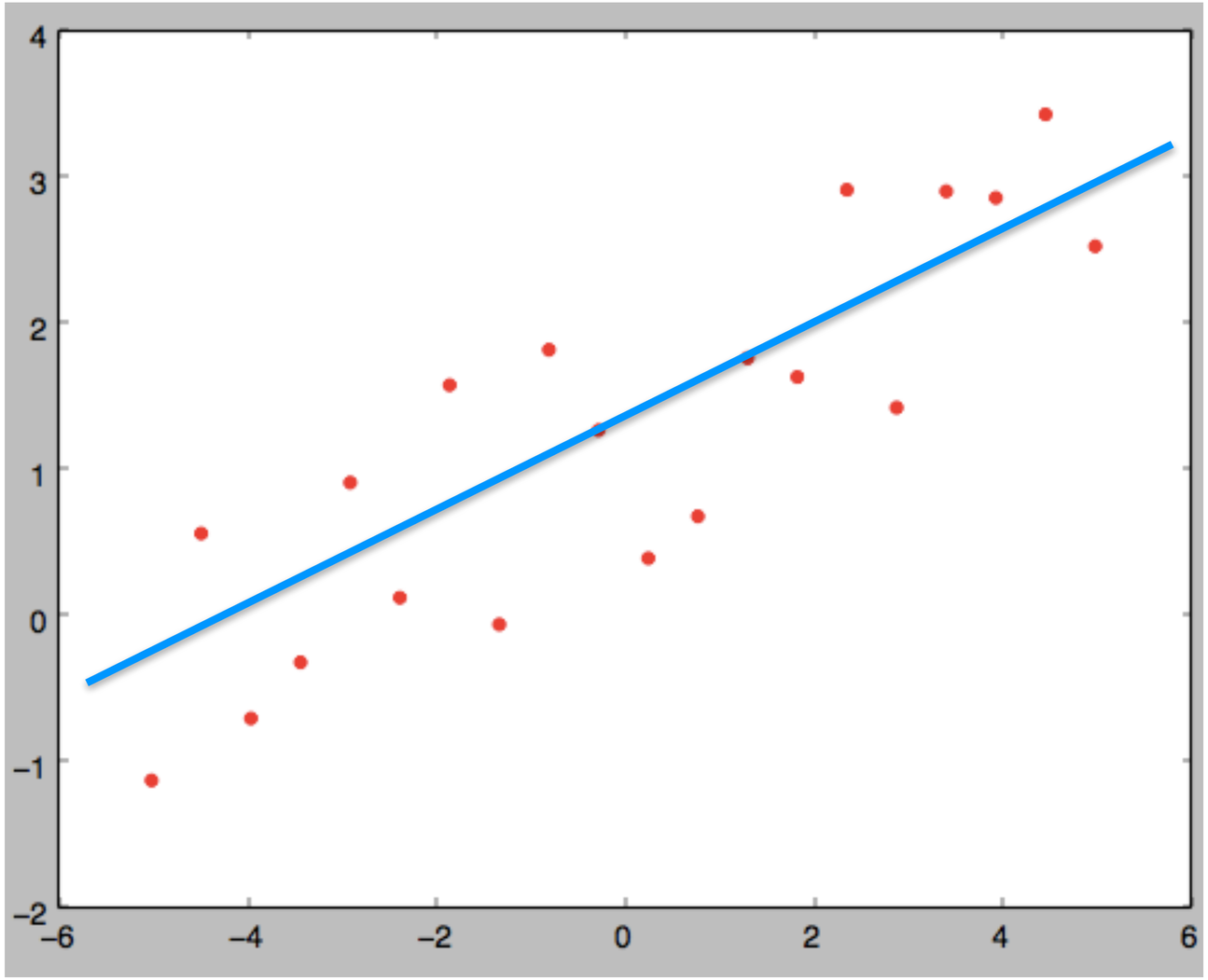
Regression: Continuous Output



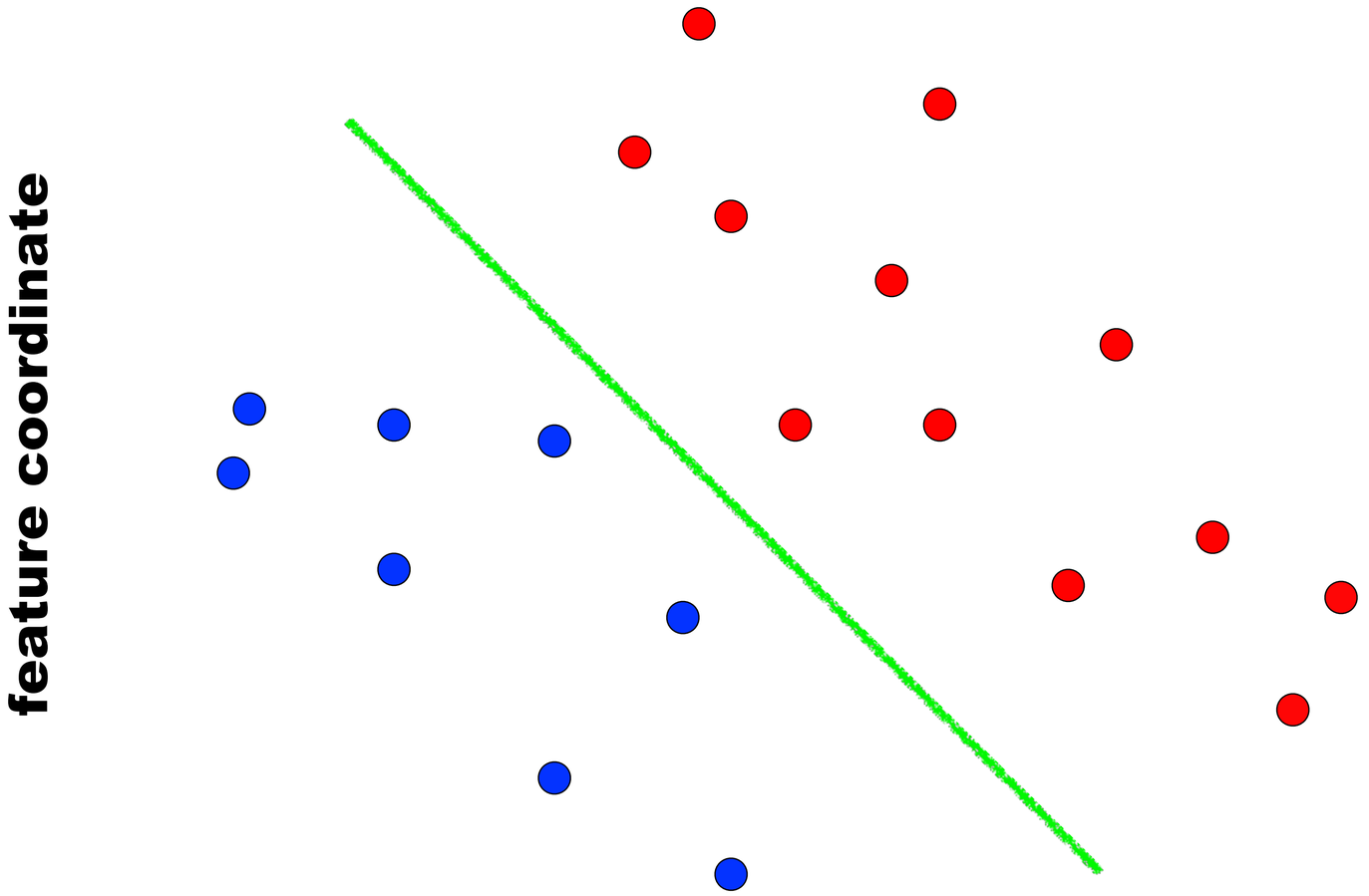
Assumption: Linear Function

$$y = f_{\mathbf{w}}(\mathbf{x}) = f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x}$$

$$\mathbf{w}^T \mathbf{x} = \langle \mathbf{w}, \mathbf{x} \rangle = \sum_{d=1}^{D} \mathbf{w}_d \mathbf{x}_d$$

$$\mathbf{x} \in \mathbb{R}^D, \mathbf{w} \in \mathbb{R}^D$$

Reminder: Linear Classifier



$\mathbf{x}_i$ positive: $\mathbf{x}_i \cdot \mathbf{w} \geq 0$

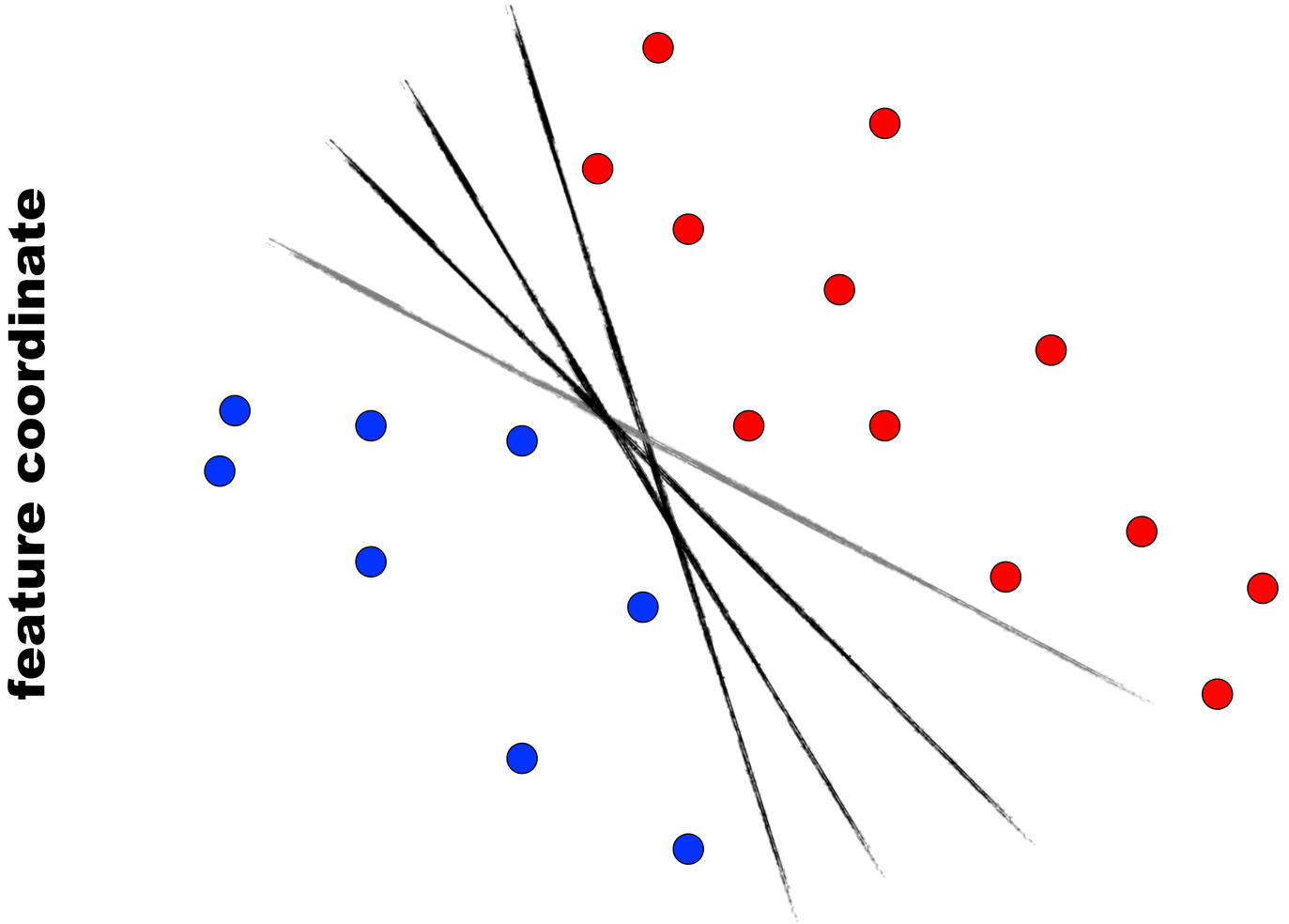
$\mathbf{x}_i$ negative: $\mathbf{x}_i \cdot \mathbf{w} < 0$

supervised setting

labelled input

$$y_t = \begin{cases} +1 & \bullet \\ -1 & \bullet \end{cases}$$

Which Line to Pick?



$\mathbf{x}_i$ positive: $\mathbf{x}_i \cdot \mathbf{w} \geq 0$

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supervised setting

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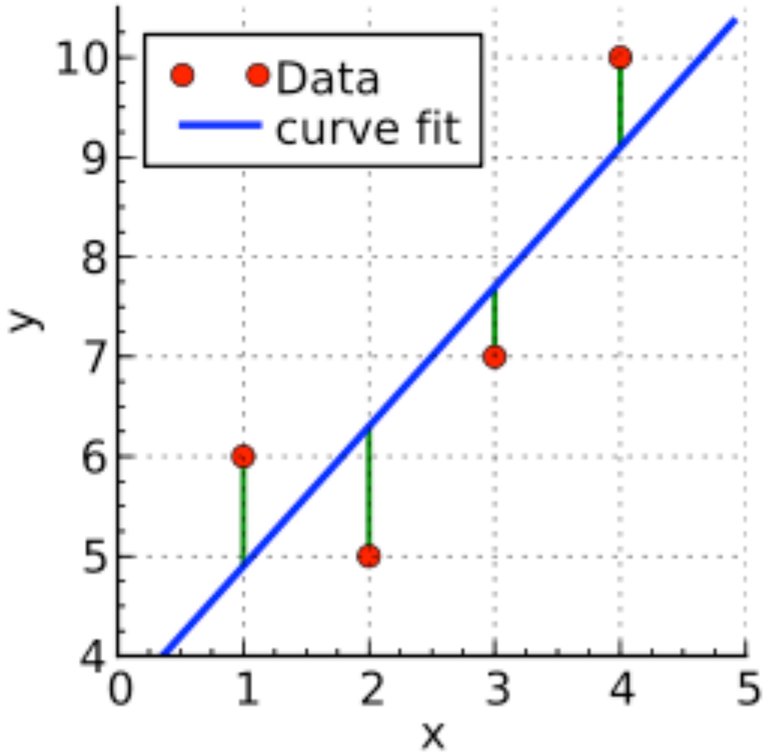
Linear Regression in 1D



Training set:
input–output pairs

$$\mathcal{S} = \{(x^i, y^i)\}, \quad i = 1 \ldots, N$$

$$x^i \in \mathbb{R}, \quad y^i \in \mathbb{R}$$

Linear regression in 1D

$$y^i = w_0 + w_1 x_1^i + \epsilon^i$$

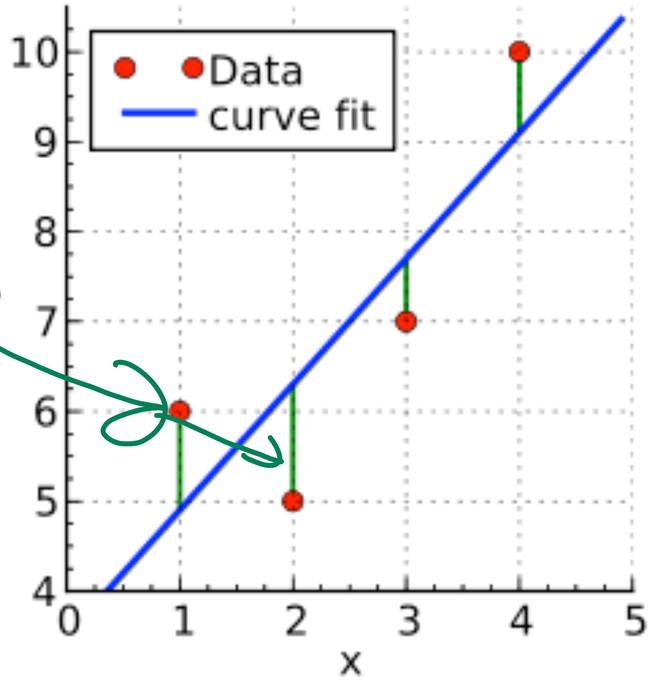
w_0 bias

$$= w_0 x_0^i + w_1 x_1^i + \epsilon^i, \quad x_0^i = 1, \quad \forall i$$

$$= \mathbf{w}^T \mathbf{x}^i + \epsilon^i$$

noise

green vector



Sum of Square Errors (MSE without the mean)

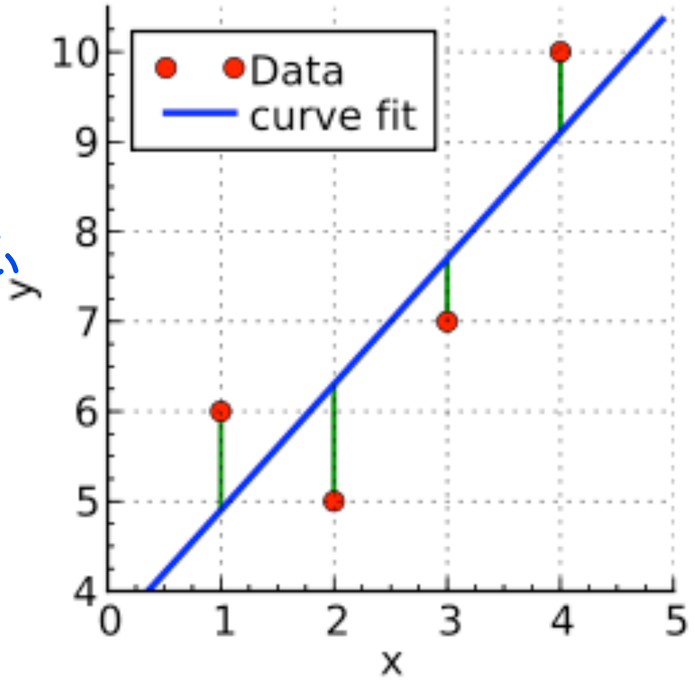
$$y^i = \mathbf{w}^T \mathbf{x}^i + \epsilon^i$$

Loss function: sum of squared errors

$$L(\mathbf{w}) = \sum_{i=1}^{N} (\epsilon^i)^2$$

In two variables:

$$L(w_0, w_1) = \sum_{i=1}^{N} \left[y^i - \left(w_0 x_0^i + w_1 x_1^i \right) \right]^2$$



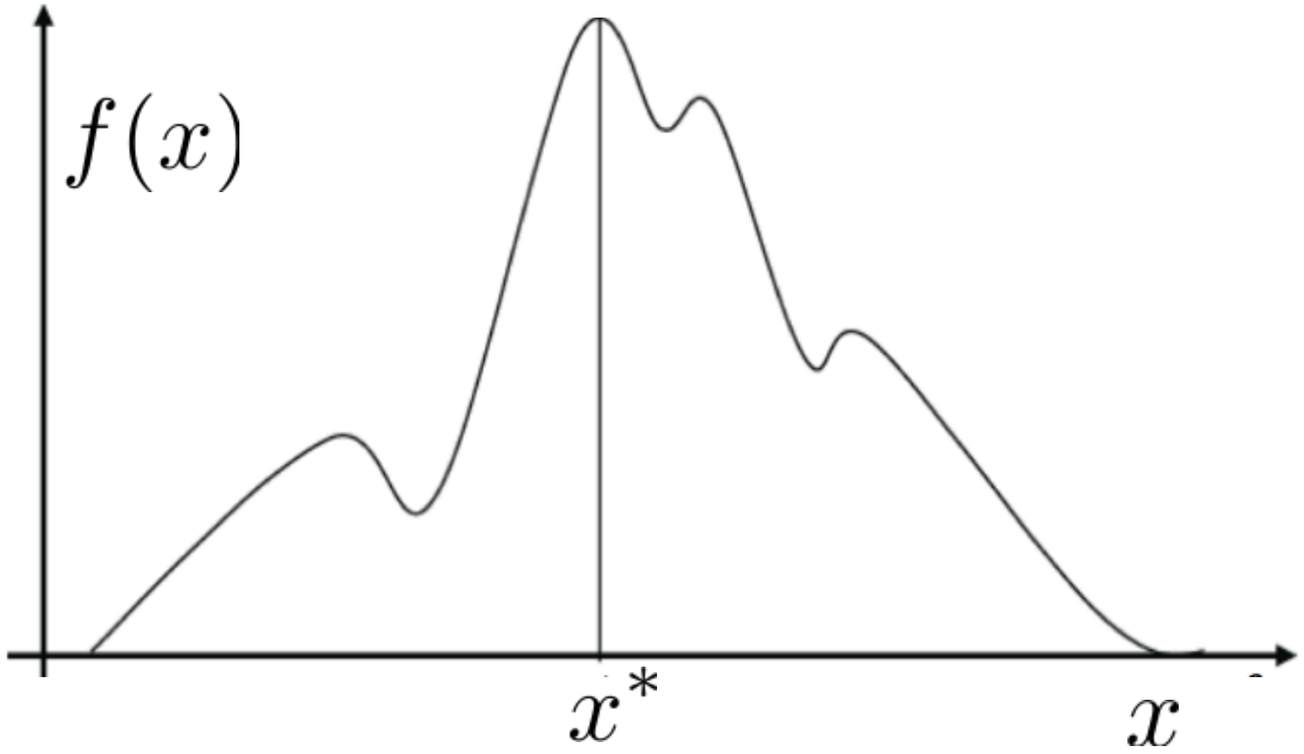
Question: what is the best (or least bad) value of w?

Line Fitting

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

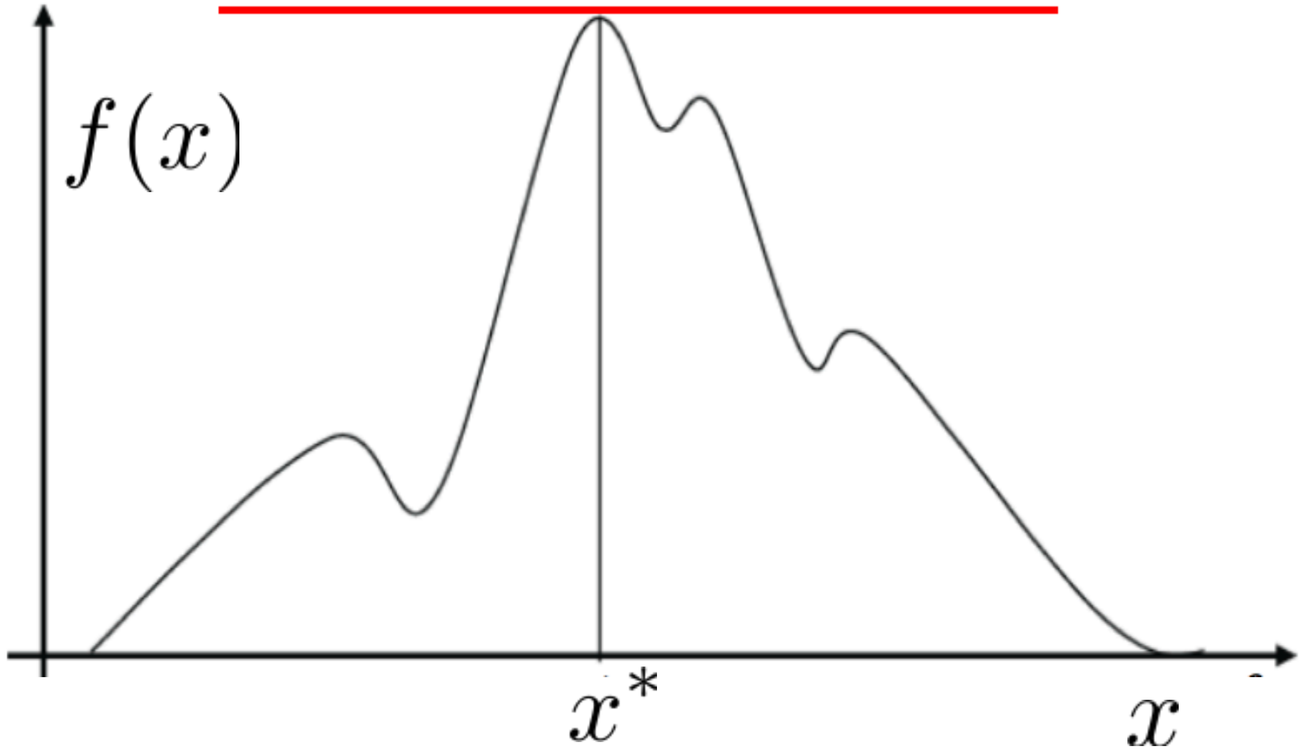
$$\mathbf{X} = \begin{bmatrix} x_0^1 & x_1^1 \\ \vdots & \vdots \\ x_0^N & x_1^N \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y^1 \\ \vdots \\ y^N \end{bmatrix}$$

Calculus 101



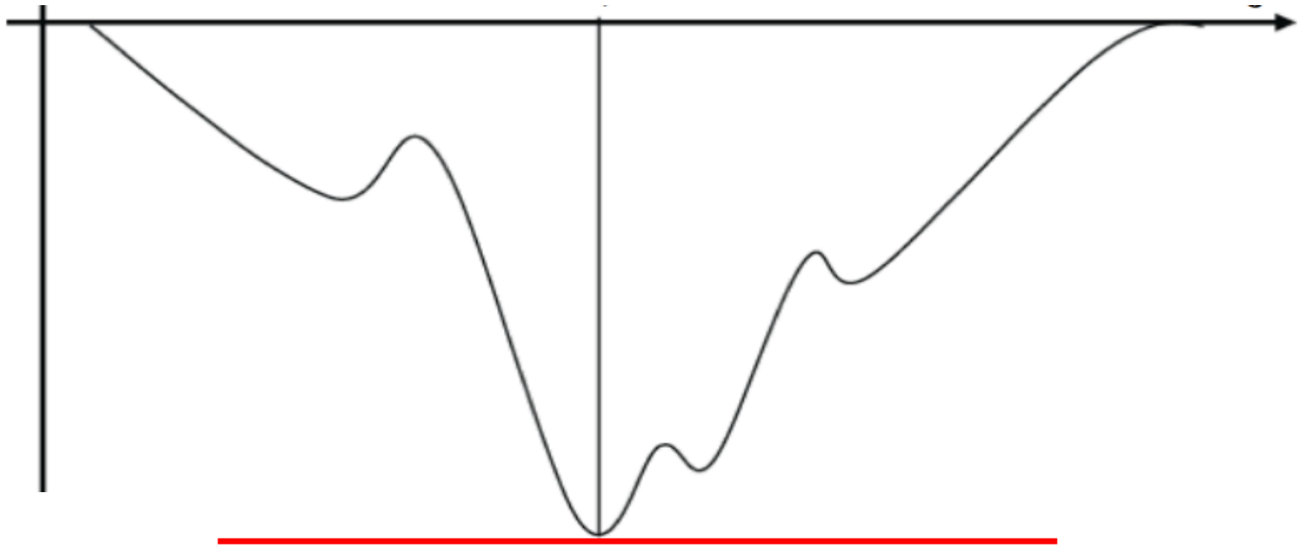
$$x^* = \text{argmax}_x f(x)$$

Local Extrema Condition



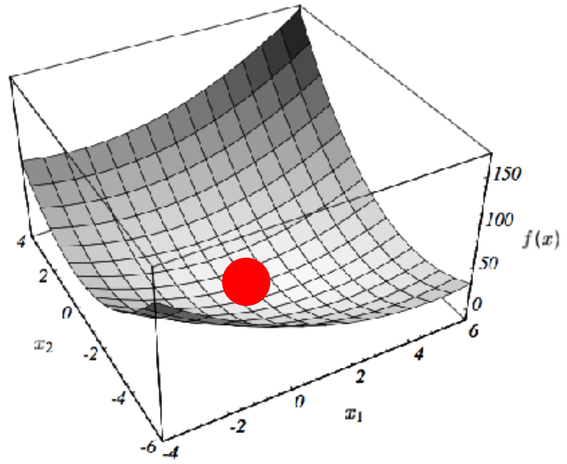
$$x^* = \text{argmax}_x f(x) \quad \rightarrow \quad f'(x^*) = 0$$

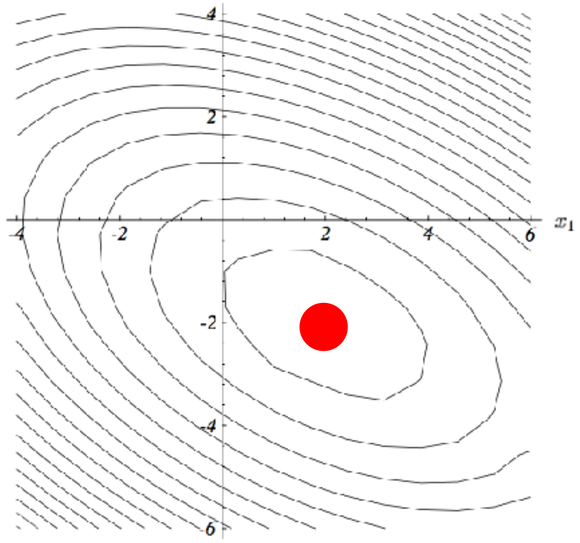
Local Extrema Condition

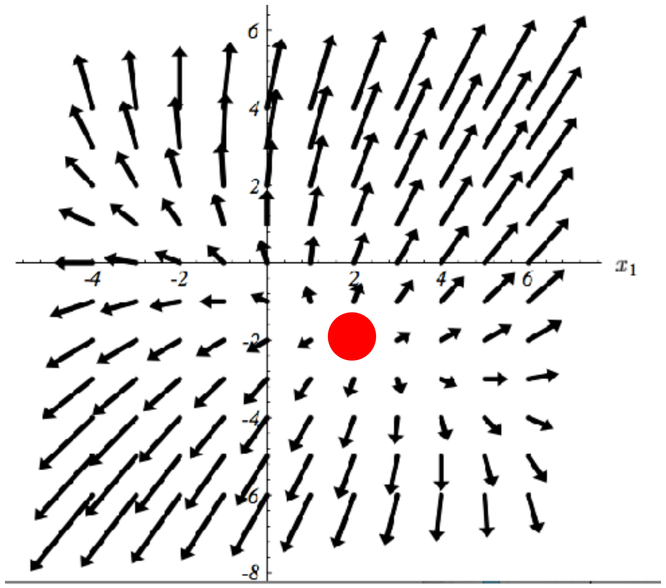


$$x^* = \text{argmax}_x f(x) \quad \rightarrow \quad f'(x^*) = 0$$

Vector Calculus 101







$$f(\mathbf{x})$$

$$f(\mathbf{x}) = c$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

2D function graph **isocontours** **gradient field**

- **at minimum of function:** $\nabla f(\mathbf{x}) = 0$

Line Fitting

$$L(w_0, w_1) = \sum_{i=1}^{N} \left[y^i - \left(w_0 x_0^i + w_1 x_1^i \right) \right]^2$$

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = \sum_{i=1}^{N} \frac{\partial \left[y^i - \left(w_0 x_0^i + w_1 x_1^i \right) \right]^2}{\partial w_0}$$

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = \sum_{i=1}^{N} \frac{\partial [z^i]^2}{\partial z^i} \frac{\partial z^i}{\partial w_0} = \sum_{i=1}^{N} (2z^i)(-x_0^i)$$

$$= -2 \sum_{i=1}^{N} (y^i - (w_0 x_0^i + w_1 x_1^i)) x_0^i$$

$$z^i = y^i - (w_0 x_0^i + w_1 x_1^i)$$

Line Fitting (continued)

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = \sum_{i=1}^{N} \frac{\partial \left[y^i - \left(w_0 x_0^i + w_1 x_1^i \right) \right]^2}{\partial w_0}$$

$$= -2 \sum_{i=1}^{N} \left(y^i x_0^i - w_0 x_0^i x_0^i - w_1 x_1^i x_0^i \right)$$

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = 0$$

$$\sum_{i=1}^{N} y^i x_0^i = w_0 \sum_{i=1}^{N} x_0^i x_0^i + w_1 \sum_{i=1}^{N} x_1^i x_0^i$$

Line Fitting (continued)

$$\sum_{i=1}^{N} y^i x_0^i = w_0 \sum_{i=1}^{N} x_0^i x_0^i + w_1 \sum_{i=1}^{N} x_1^i x_0^i$$

$$\sum_{i=1}^{N} y^i x_1^i = w_0 \sum_{i=1}^{N} x_0^i x_1^i + w_1 \sum_{i=1}^{N} x_1^i x_1^i$$

2x2 system of equations

$$\begin{bmatrix} \sum_{i=1}^{N} y^i x_0^i \\ \sum_{i=1}^{N} y^i x_1^i \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} x_0^i x_0^i & \sum_{i=1}^{N} x_0^i x_1^i \\ \sum_{i=1}^{N} x_0^i x_1^i & \sum_{i=1}^{N} x_1^i x_1^i \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

Line Fitting (continued)

$$\begin{bmatrix} \sum_{i=1}^{N} y^i x_0^i \\ \sum_{i=1}^{N} y^i x_1^i \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} x_0^i x_0^i & \sum_{i=1}^{N} x_0^i x_1^i \\ \sum_{i=1}^{N} x_0^i x_1^i & \sum_{i=1}^{N} x_1^i x_1^i \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

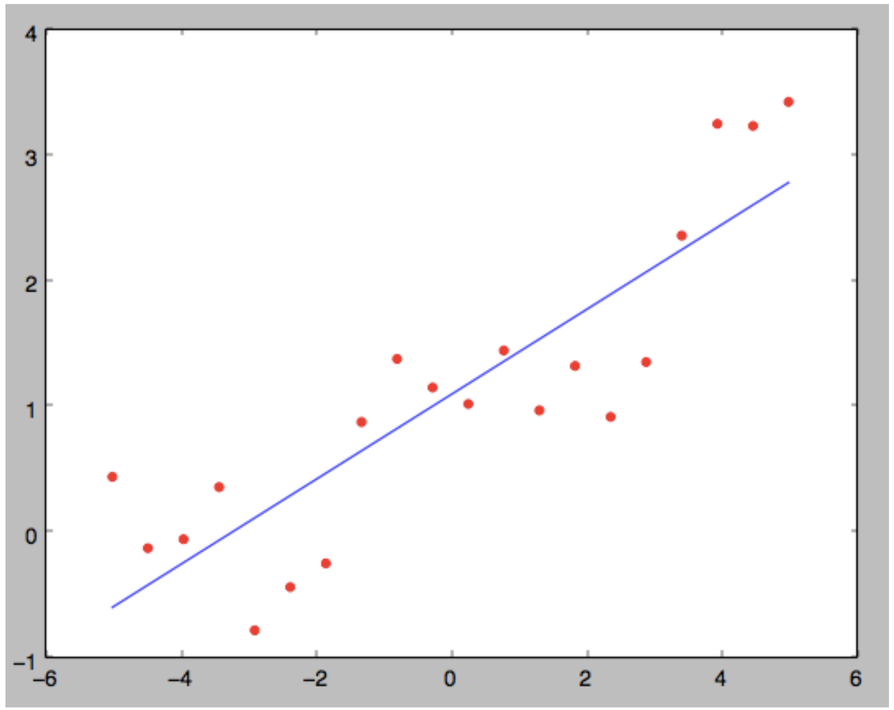
$$\mathbf{X}^T\mathbf{y} = \mathbf{X}^T\mathbf{X}\mathbf{w}$$

$$\mathbf{y} = \begin{bmatrix} y^1 \\ \vdots \\ y^N \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} x_0^1 & x_1^1 \\ \vdots & \vdots \\ x_0^N & x_1^N \end{bmatrix}$$

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Normal Equation

Code Example




```python
import numpy as np
from numpy import array
from numpy import matmul
from numpy.linalg import inv
from numpy.random import rand
from matplotlib import pyplot

# generate data on a line perturbed with some noise
noise_margin= 2
w = rand(2,1) # w[0] is random constant term (offset from origin), w[1] is random linear term (slope)
x  = np.linspace(-5,5,20)
y = w[0] + w[1]*x + noise_margin*rand(len(x))

# create the design matrix: the x data, and add a column of ones for the constant term
X = np.column_stack( [np.ones([len(x), 1]), x.reshape(-1, 1)] )

# These are the normal equations in matrix form: w = (X' X)^-1 X' y
w_est = matmul(inv(matmul(X.transpose(),X)),X.transpose()).dot(y)

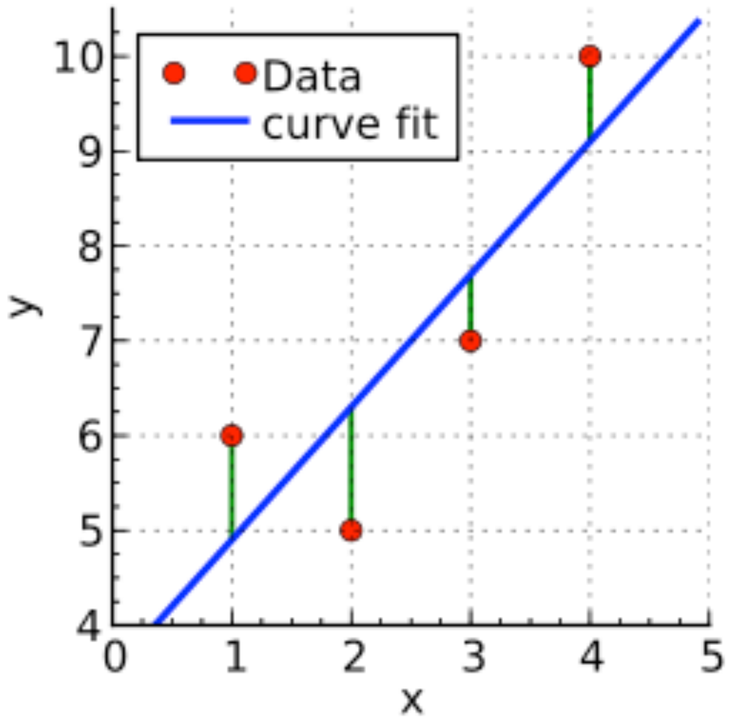
# For ridge regression, use regularizer
#weight = 0.01
#w_est = matmul(inv(matmul(X.transpose(),X) + weight*np.identity(2)),X.transpose()).dot(y)

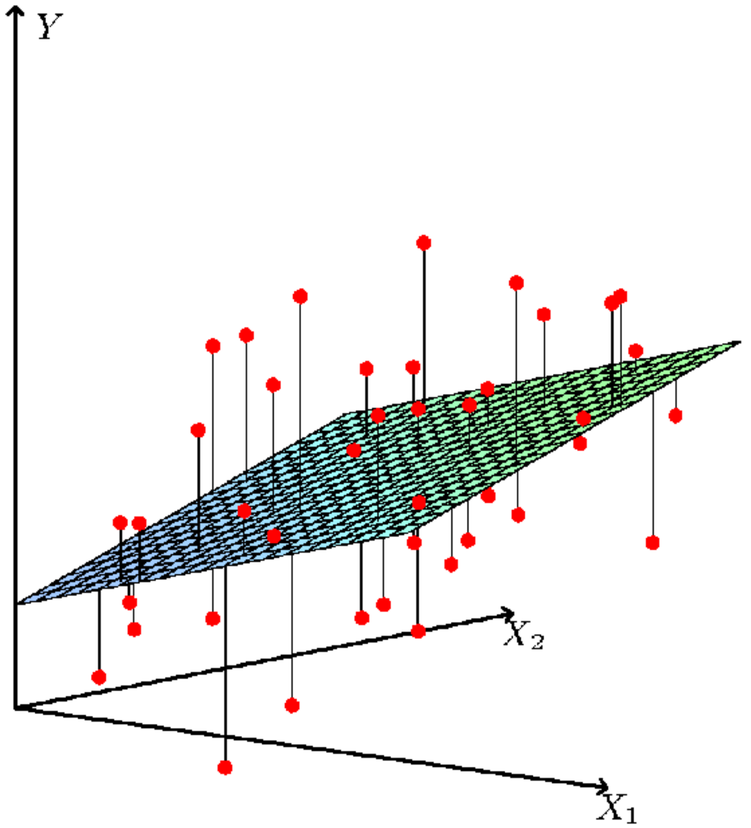

# evaluate the x values in the fitted model to get estimated y values
y_est = w_est[0] + w_est[1]*x

# visualize the fitted model
pyplot.scatter(x, y, color='red')
pyplot.plot(x, y_est, color='blue')
pyplot.show()
```

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Linear Regression (Line/Plane Fitting)





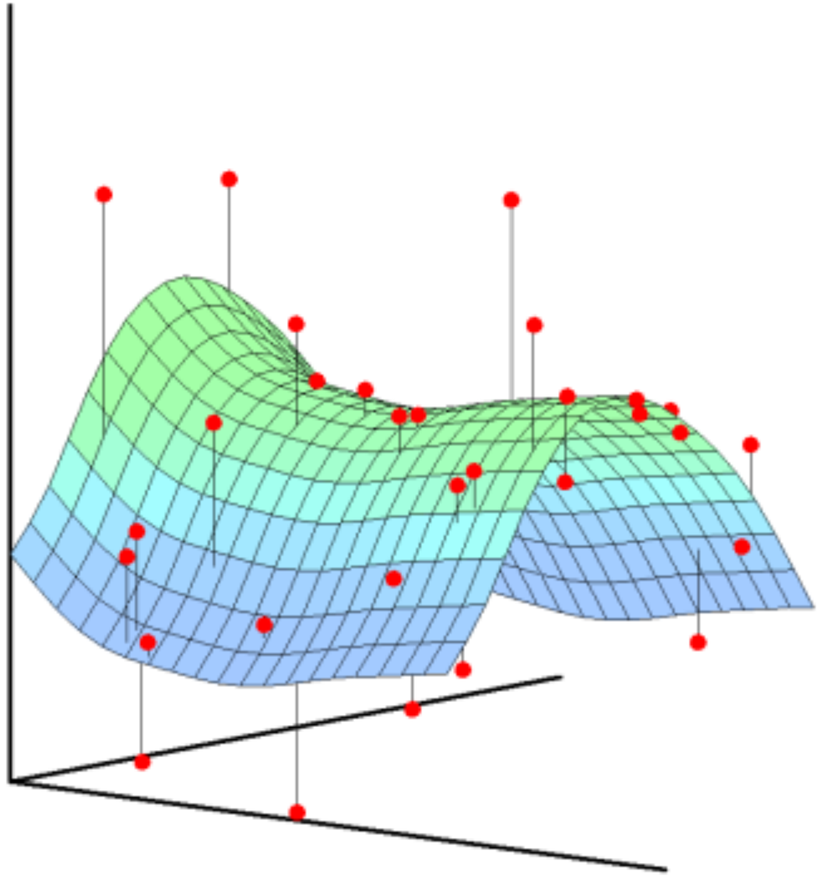
LS Solution for Regression

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^T \mathbf{x}^i)^2 = \sum_{i=1}^{N} (\epsilon^i)^2$$

$$L(\mathbf{w}) = \begin{bmatrix} \epsilon^1 & \epsilon^2 & \dots & \epsilon^N \end{bmatrix} \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} \qquad \mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\epsilon}$$

Generalized Linear Regression

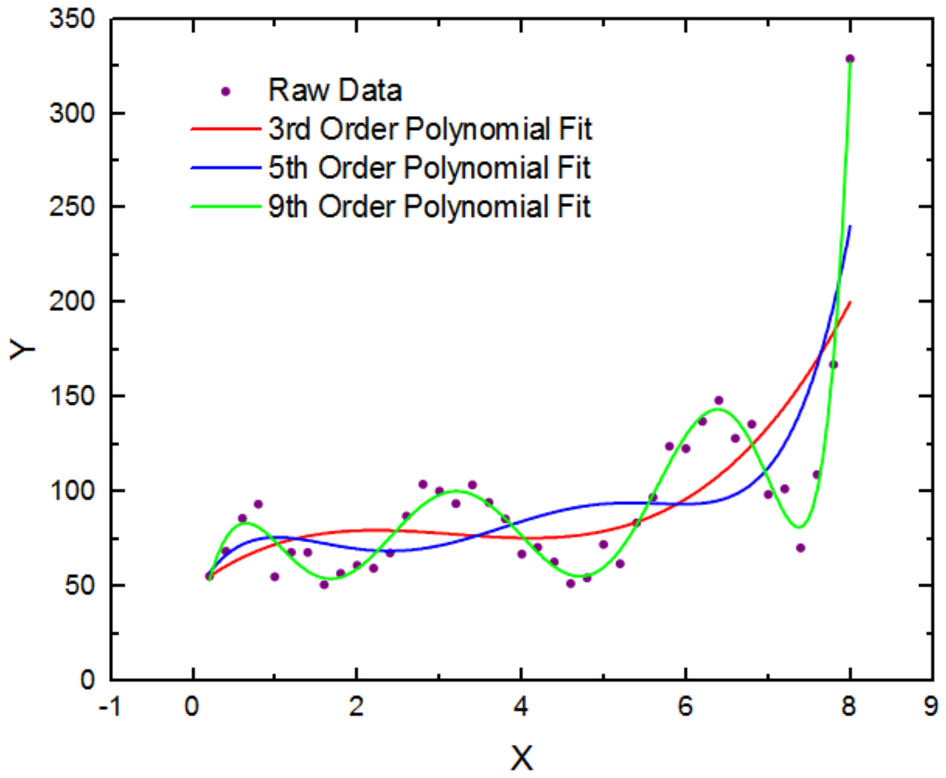


$$\mathbf{x} \rightarrow \boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \phi_1(\mathbf{x}) \\ \vdots \\ \phi_M(\mathbf{x}) \end{bmatrix}$$

known nonlinearity

1D Example: k-th Degree Polynomial Fitting

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x \\ \vdots \\ (x)^K \end{bmatrix}$$



$$\langle \mathbf{w}, \boldsymbol{\phi}(x) \rangle = w_0 + w_1 x + \ldots + w_k (x)^K$$

Generalized Linear Regression

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}^i))^T = \sum_{i=1}^{N} (\epsilon^i)^2$$

$$\begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^N \end{bmatrix} = \begin{bmatrix} \boldsymbol{\phi}(\mathbf{x}^1)^T \\ \hline \boldsymbol{\phi}(\mathbf{x}^2)^T \\ \hline \vdots \\ \hline \boldsymbol{\phi}(\mathbf{x}^N)^T \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_M \end{bmatrix} + \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

Nx1 **NxM** **Mx1** **Nx1**

$$\boldsymbol{\phi}(\mathbf{x}) : \mathbb{R}^D \rightarrow \mathbb{R}^M$$

LS Solution for Linear Regression

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\epsilon}$$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon}$$

$$\mathbf{X} = \begin{bmatrix} \frac{(\mathbf{x}^1)^T}{(\mathbf{x}^2)^T} \\ \vdots \\ \frac{}{(\mathbf{x}^N)^T} \end{bmatrix}$$

$$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

LS Solution for Generalized Linear Regression

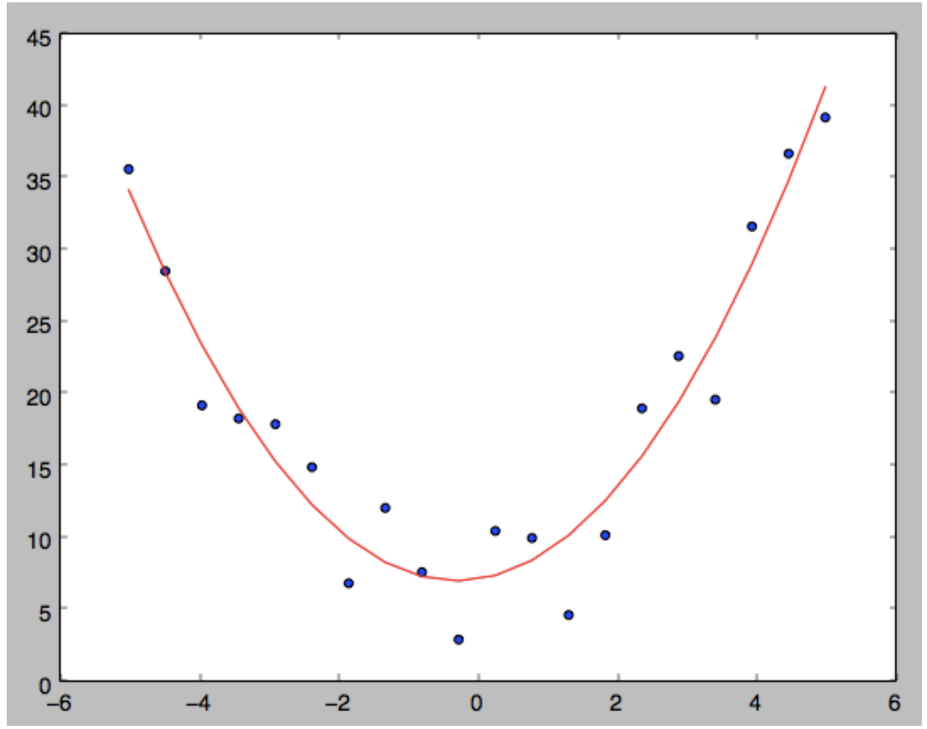
$$\mathbf{y} = \mathbf{\Phi}\mathbf{w} + \boldsymbol{\epsilon}$$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T\boldsymbol{\epsilon}$$

$$\mathbf{\Phi} = \begin{bmatrix} \boldsymbol{\phi}(\mathbf{x}^1)^T \\ \hline \boldsymbol{\phi}(\mathbf{x}^2)^T \\ \hline \vdots \\ \hline \boldsymbol{\phi}(\mathbf{x}^N)^T \end{bmatrix}$$

$$\mathbf{w}^* = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}\mathbf{y}$$

Code Example

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# generate data on a line perturbed with some noise
noise_margin= 3
w = 2*rand(3,1) # w[0] is random constant term (offset from origin), w[1] is random linear term, w[2] is random quadratic term
x  = np.linspace(-5,5,20)
y = w[0] + w[1]*x + w[2]*x**2 + noise_margin*rand(len(x))

# create the design matrix: the x data, and add a column of ones for the constant term
X = np.column_stack( [np.ones([len(x), 1]), x.reshape(-1, 1), (x**2).reshape(-1, 1)] )

# These are the normal equations in matrix form: w = (X' X)^-1 X' y
w_est = matmul(inv(matmul(X.transpose(),X)),X.transpose()).dot(y)


# evaluate the x values in the fitted model to get estimated y values
y_est = w_est[0] + w_est[1]*x + w_est[2]*x**2

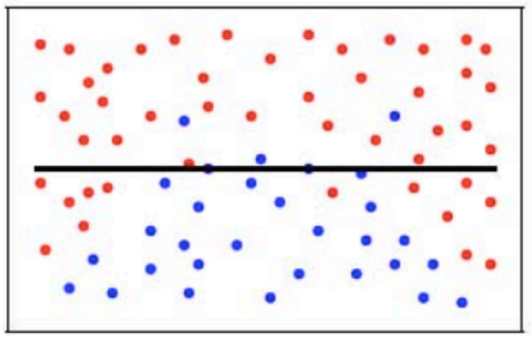
# visualize the fitted model
pyplot.scatter(x, y)
pyplot.plot(x, y_est, color='red')
pyplot.show()
```

$$\mathbf{w}^* = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}\mathbf{y}$$

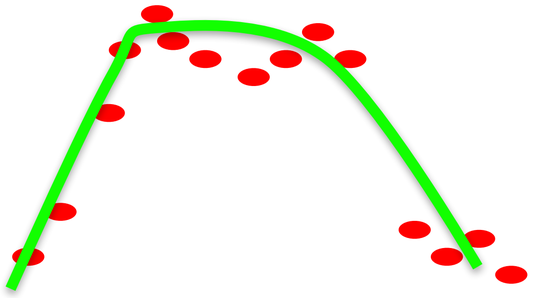
Underfitting vs. Overfitting

Underfitting

classification



regression



Regularized Linear Regression

$$\boldsymbol{\epsilon} = \mathbf{y} - \boldsymbol{\Phi}\mathbf{w}$$

residual vector

这里Φ是X构成的矩阵

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T\boldsymbol{\epsilon}$$

linear regression: minimize model error

Complexity term: (regularizer)

$$R(\mathbf{w}) \doteq \|\mathbf{w}\|_2^2 = \mathbf{w}^T\mathbf{w}$$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T\boldsymbol{\epsilon} + \lambda\mathbf{w}^T\mathbf{w}$$

"data fidelity" **complexity**

minimum remains to be determined

scalar, remains to be determined

Least Squares Solution

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon}$$
$$= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$
$$= \mathbf{y}^T\mathbf{y} - 2\mathbf{y}^T\mathbf{X}\mathbf{w} + \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}$$

Condition for minimum:

$$\nabla L(\mathbf{w}^*) = \mathbf{0}$$

$$-2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\mathbf{w}^* = \mathbf{0}$$

$$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Ridge regression: L2-regularized Linear Regression

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} + \lambda \mathbf{w}^T \mathbf{w}$$

$$= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\mathbf{w} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w} + \lambda \mathbf{w}^T \mathbf{I}\mathbf{w}$$

as before, for linear regression

identity matrix

$$= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\mathbf{w} + \mathbf{w}^T \left(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}\right) \mathbf{w}$$

Condition for minimum:

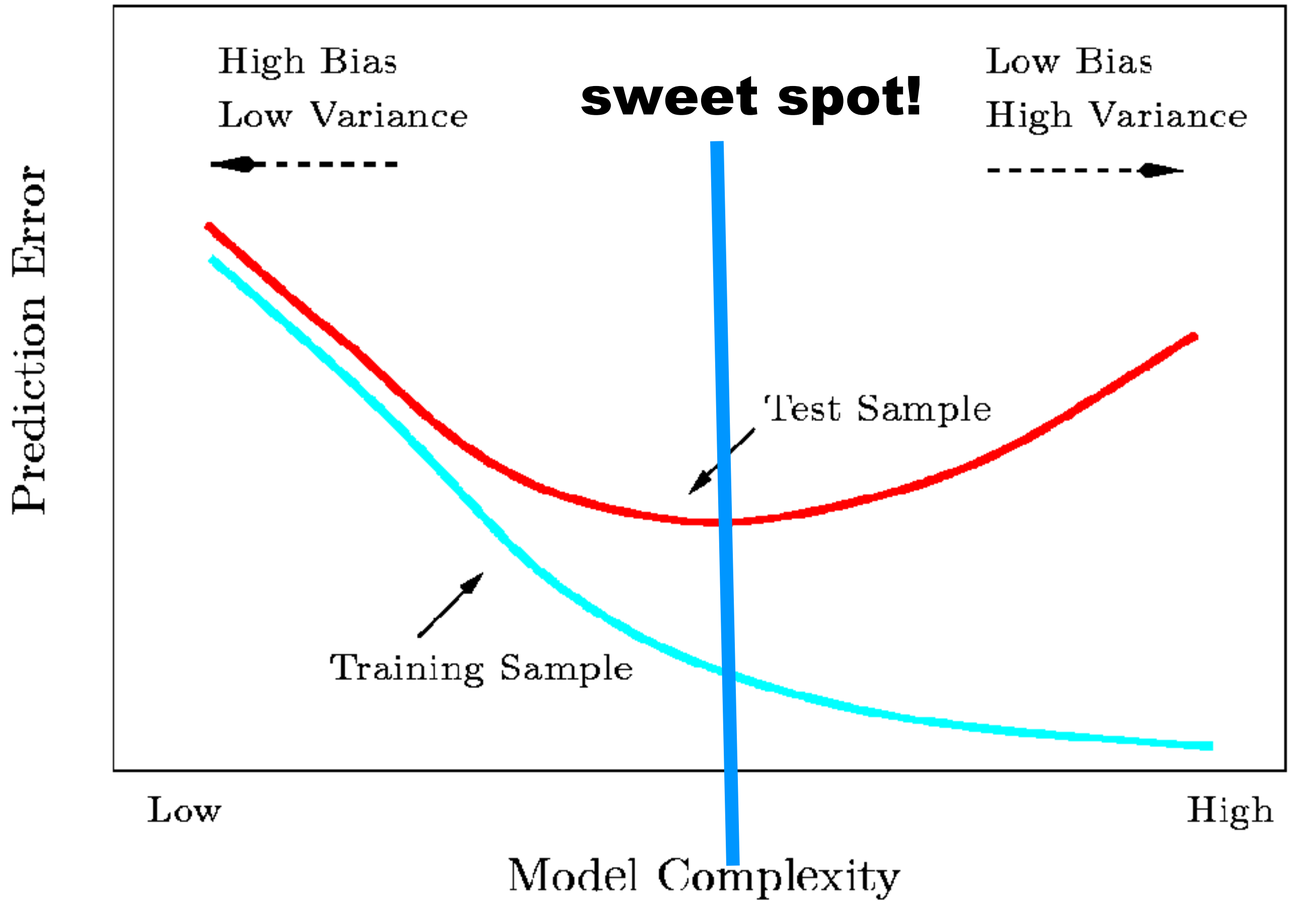
$$\nabla L(\mathbf{w}^*) = \mathbf{0}$$

$$-2\mathbf{X}^T \mathbf{y} + 2(\mathbf{X}^T \mathbf{X} + \lambda I)\mathbf{w}^* = 0$$

$$\mathbf{w}^* = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

λ: "hyperparameter"

Bias-Variance Tradeoff (function of λ)

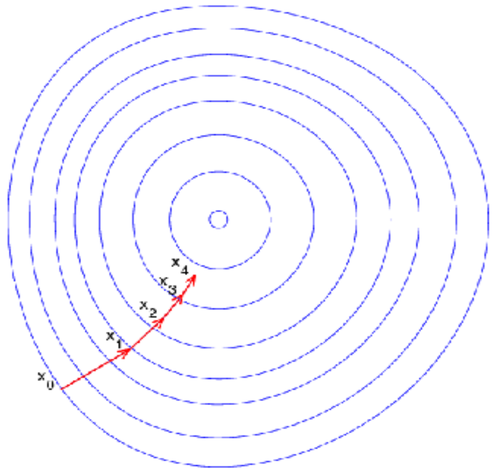


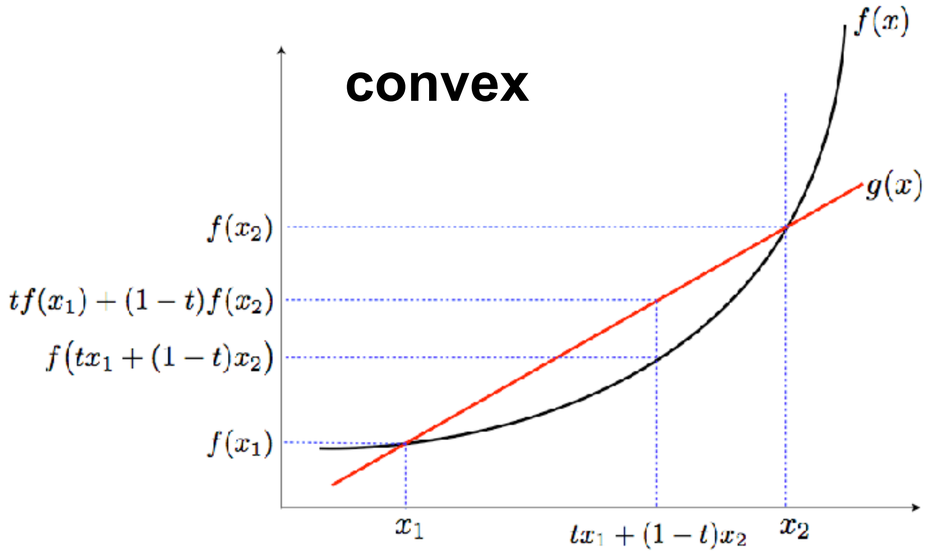
Gradient Descent Minimization

Initialize: $\mathbf{x}_0$

Update: $\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$

We can always make it converge for a convex function.





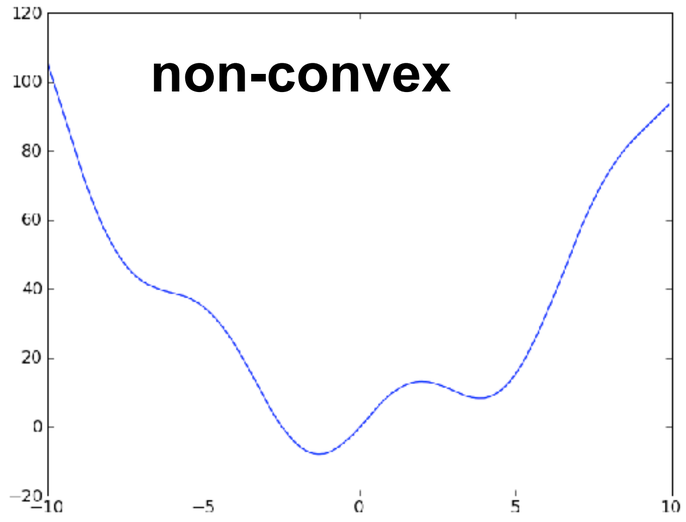


Image Classifier

- **Data (training/validation/test)** $\{\mathbf{x}_i, y_i\}$
- **Scoring function (probability of belonging to class k)** $f(\mathbf{x}_i, \mathbf{W})$
- **Loss function** $L_i(W) := h(f(\mathbf{x}_i, W), y_i) \quad L(W) := \frac{1}{N} \sum_i L_i(W)$
- **Optimization** $\mathbf{W}^* := \arg\min L(W) = \arg\min L_i(W)/N$

Linear versus Nonlinear Models

- **Objective function #1**

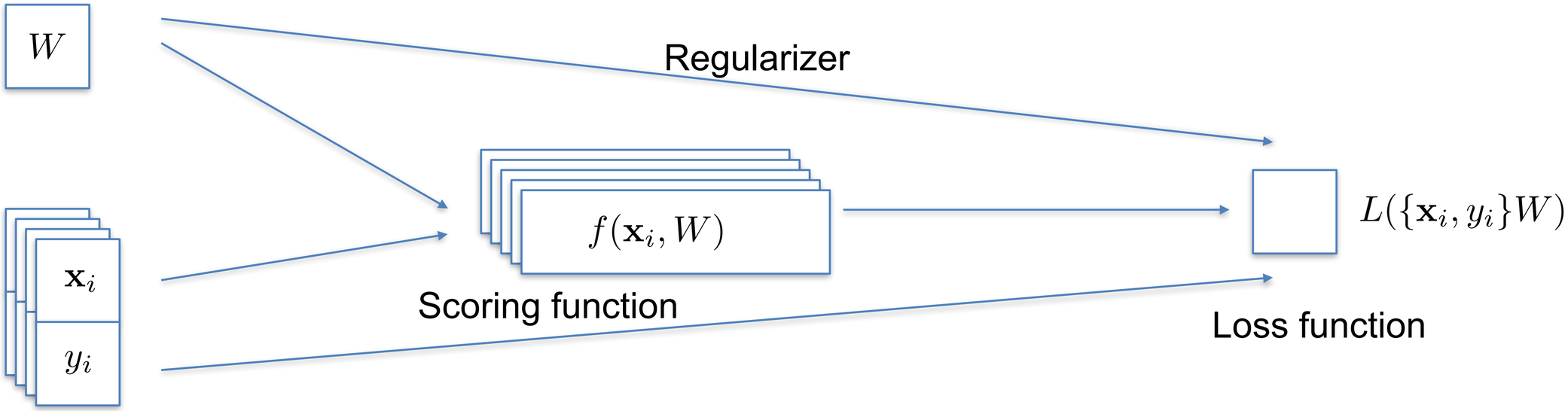
$$s = f(\mathbf{x}_i, W) = W\mathbf{x}_i$$

$$L_i(W) := (Wx_i - y_i)^2$$

- **Objective function #2**

$$L_i(W) := -\log\left(\frac{e^{Wx_iy_i}}{\sum_j e^{Wx_jy_j}}\right) = -\log\left(\frac{e^{sy_i}}{\sum_j e^{sy_j}}\right)$$

Image Classifier

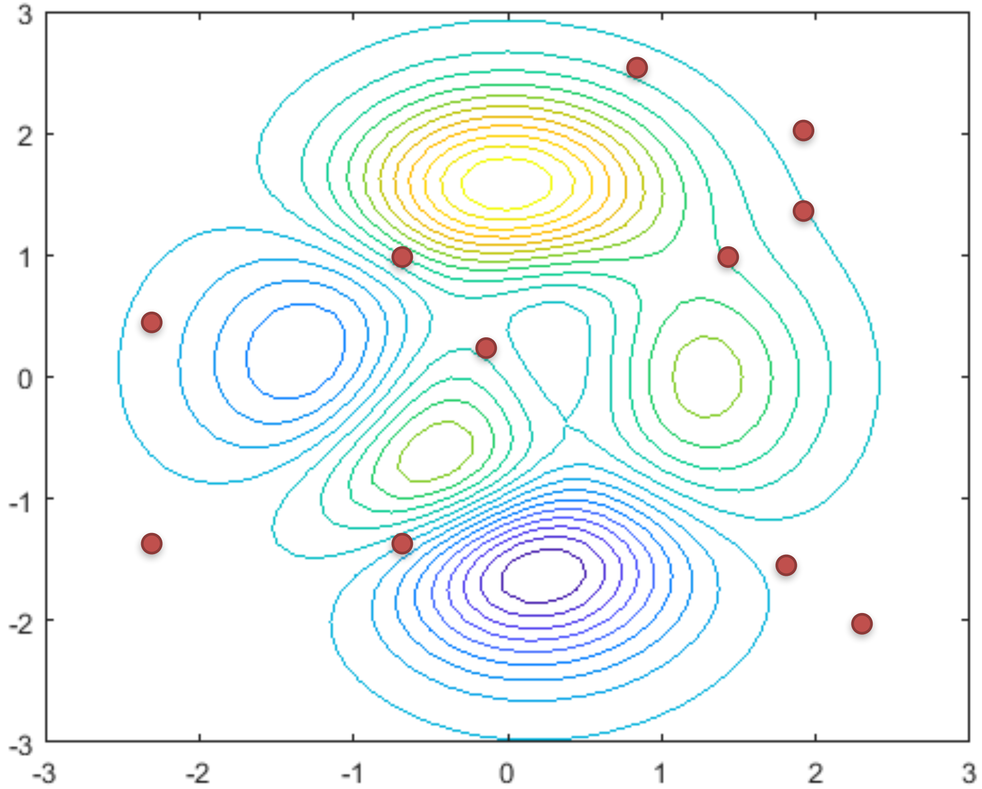


Method 1a: Random search

- `bestLoss = ∞`
- Loop

```
        Pick random W
        Compute loss
        if loss<bestLoss
              bestLoss = loss
              currW = W
         endif

  endLoop
```

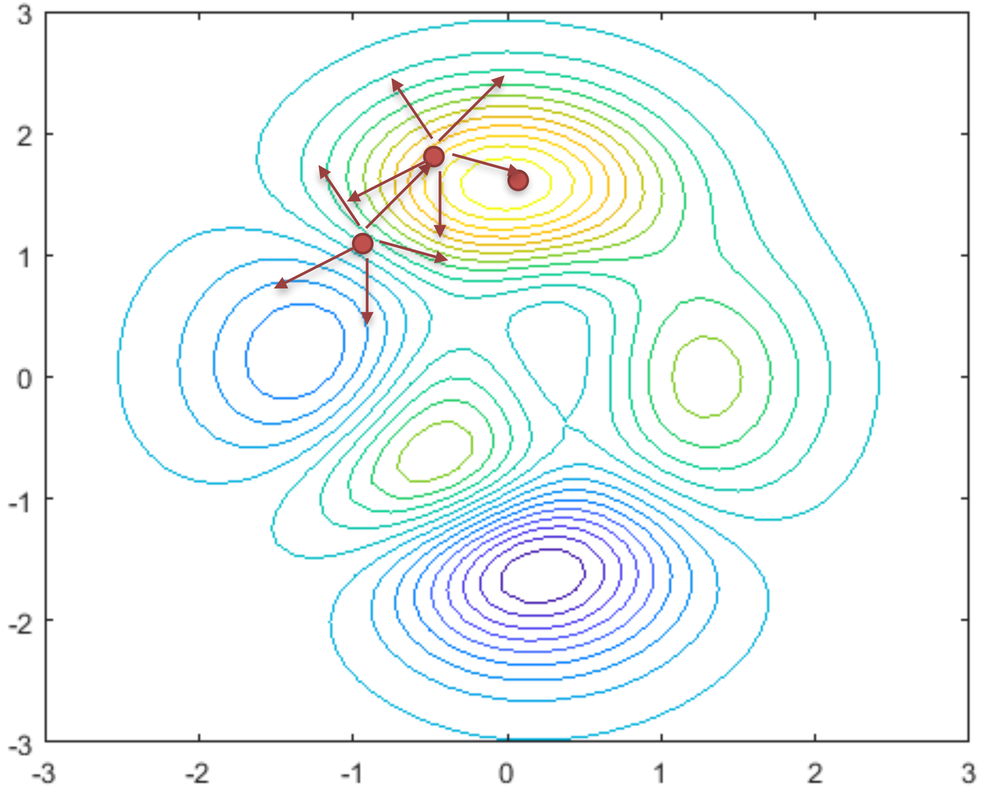


Method 1b: Random search++

- bestLoss = ∞
- W = setRand
- stepsize
- Loop

```
        W_local = W + stepsize*W_random
        Compute loss
        if loss<bestLoss
              bestLoss = loss
              W = W_local
         endif

  endLoop
```

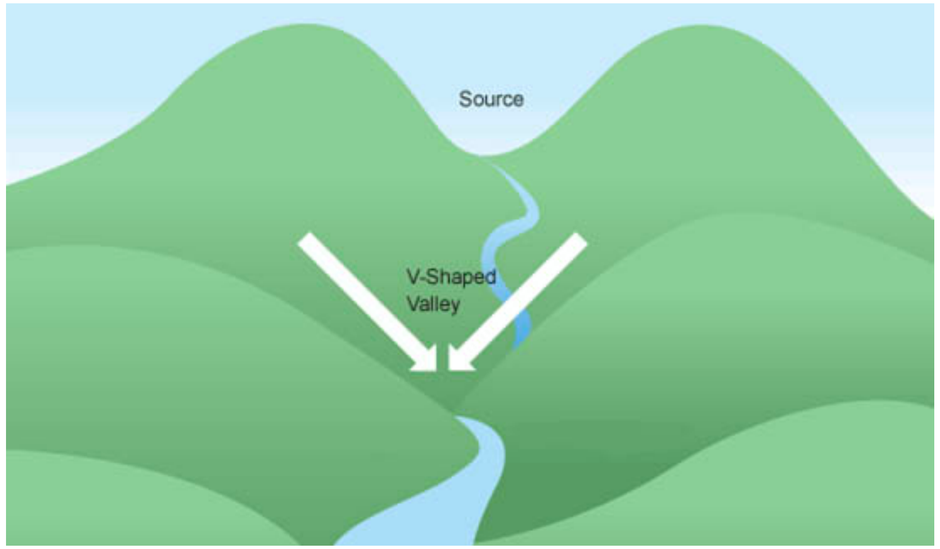


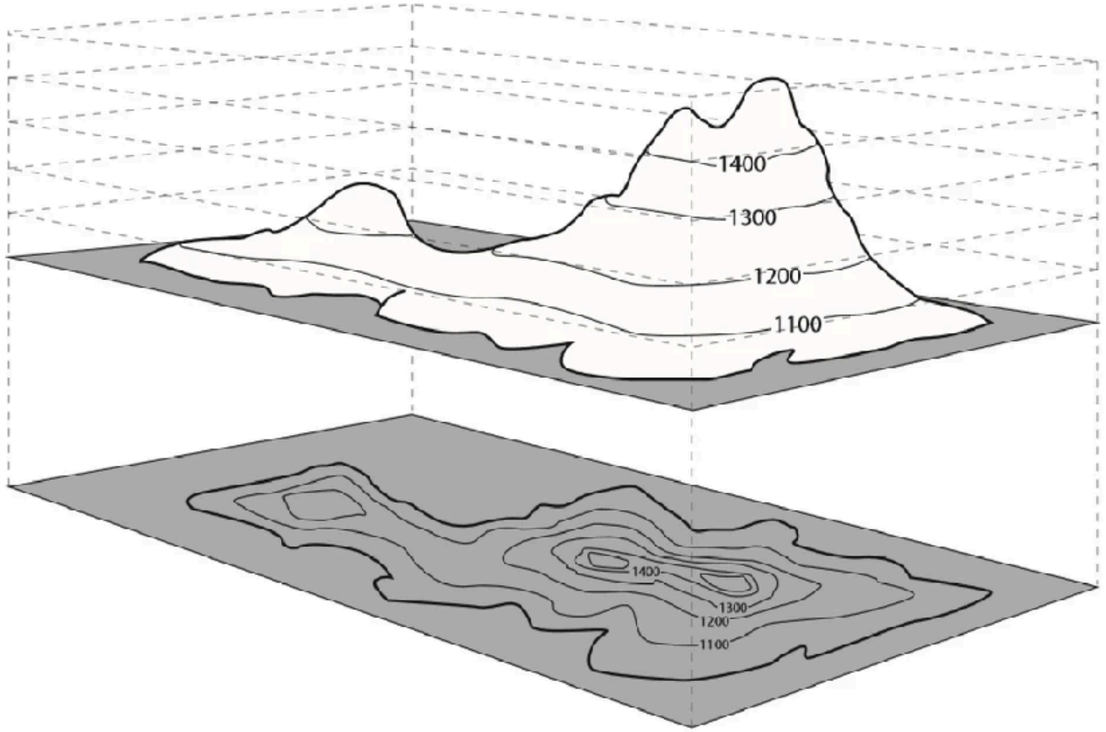
Optimize

$$\mathbf{W}^* = \arg\min g(\mathbf{x}_i, W)$$

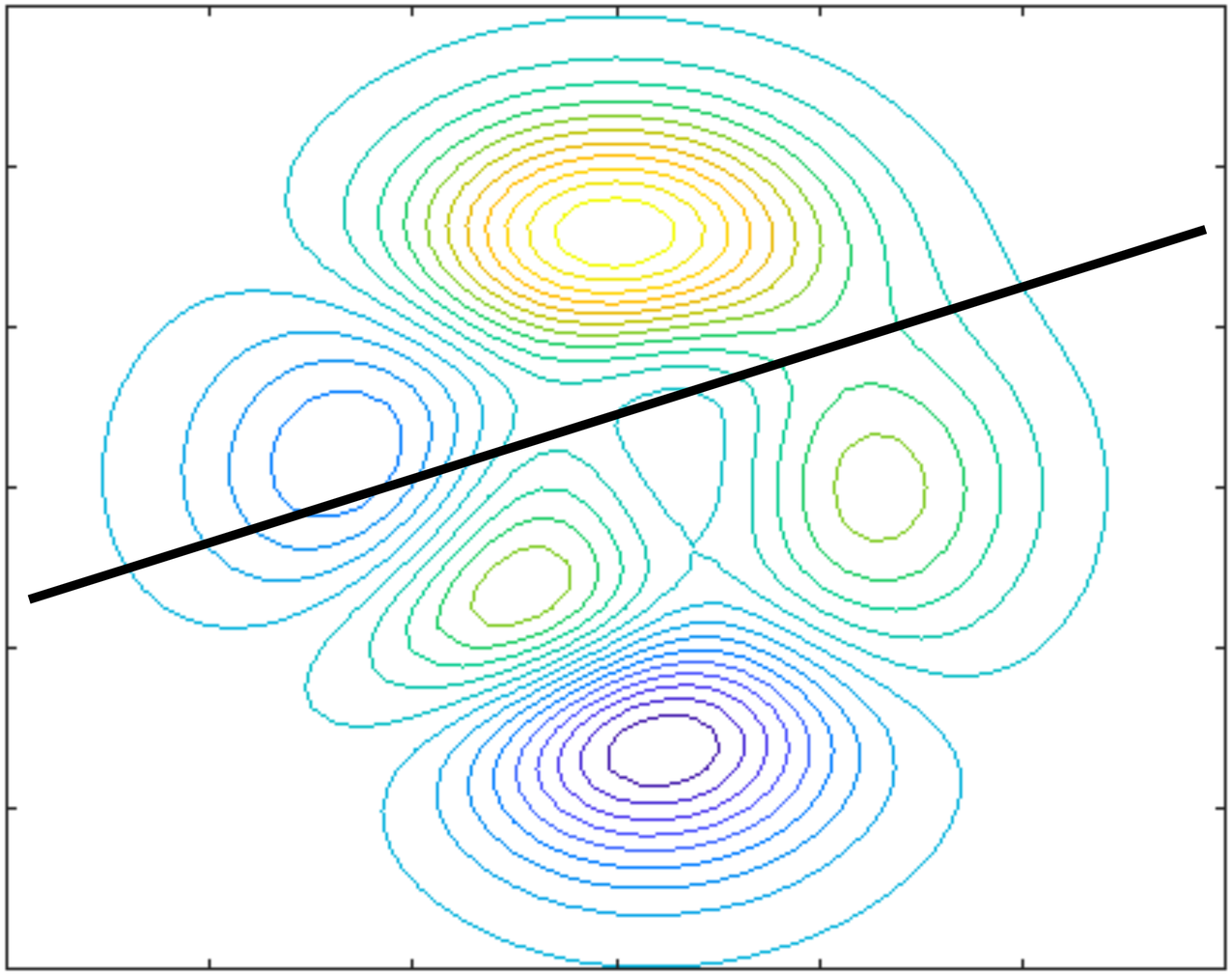
$$\nabla g(\mathbf{x}_i, W) = \left[\frac{\partial g(\mathbf{x}_i, W)}{w_i} = 0 \right]_{D \times 1}$$

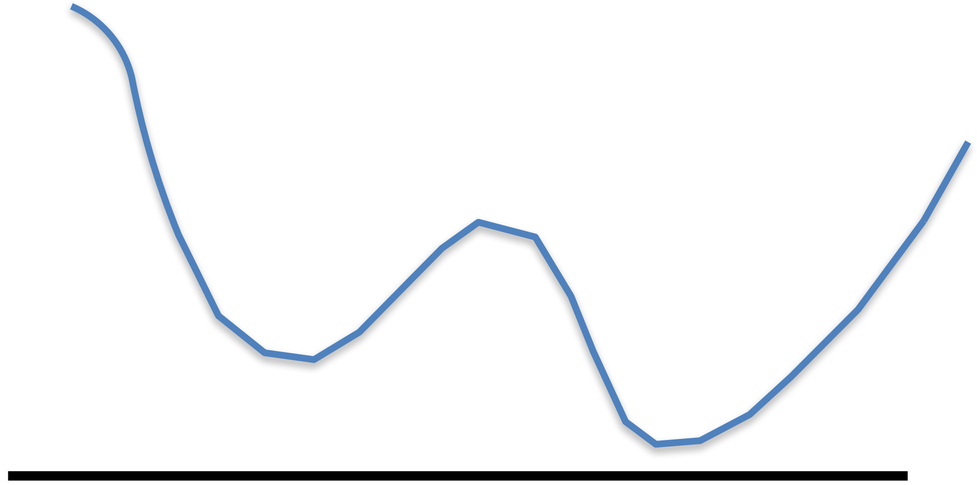
Error Landscape





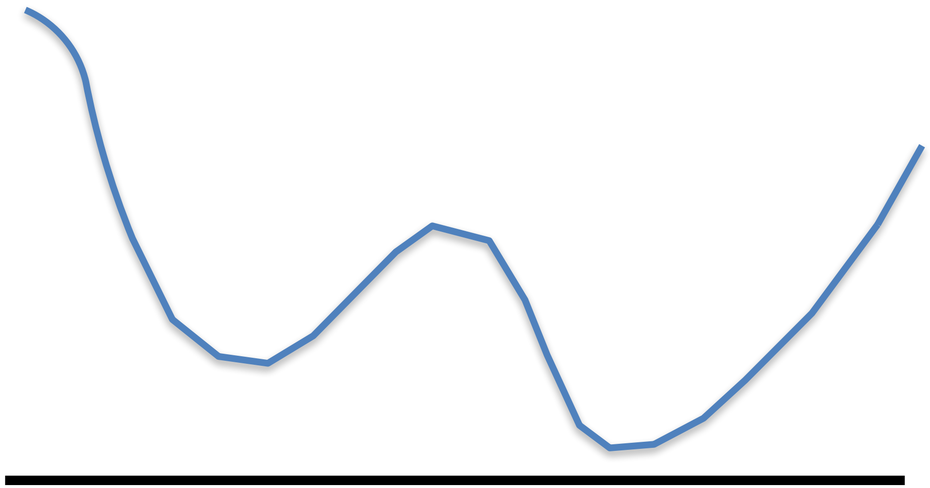
Method 2: Follow Negative of Gradient





$$\frac{df(x)}{dx}$$

Method 2: Follow Negative of Gradient



$$\frac{df(x)}{dx}$$

Compute f(x), numerically

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Stochastic Gradient Descent

$$J(\mathbf{w}) = \mathbb{E}_{\mathbf{x},y\sim p_{\text{data}}} L(\mathbf{x}, y, \mathbf{w}) = \frac{1}{N}\sum_i L(\mathbf{x}^{(i)}, y^{(i)}, \mathbf{w})$$

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \frac{1}{N}\sum_i \nabla_{\mathbf{w}} L(\mathbf{x}^{(i)}, y^{(i)}, \mathbf{w})$$

$$\nabla_{\mathbf{w}} J(\mathbf{w}) \approx \frac{1}{m}\sum_i \nabla_{\mathbf{w}} L(\mathbf{x}^{(i)}, y^{(i)}, \mathbf{w})$$

Compute f(x), numerically

0.45	0.45+0	
1.34	1.34+0	
3.26	3.26+0.0001	
-1.45	-1.45+0	
3.2	3.2+0	

Numerical vs Analytical Gradients

- Slow versus Fast
- Easy versus error-prone
- Check using numerical gradients