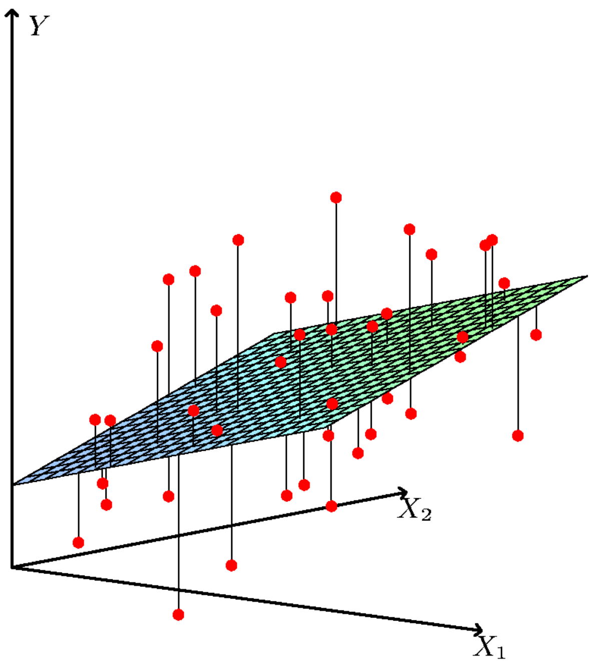
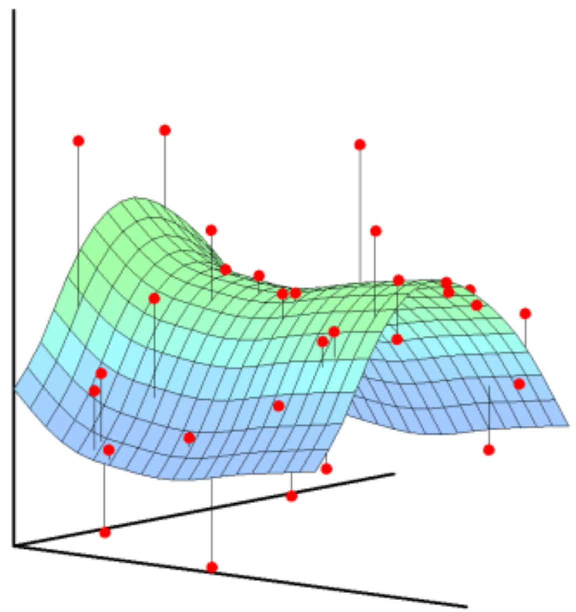
Introduction to Supervised Learning





Week 2: Maximum Likelihood Parameter Estimation,
Linear Regression

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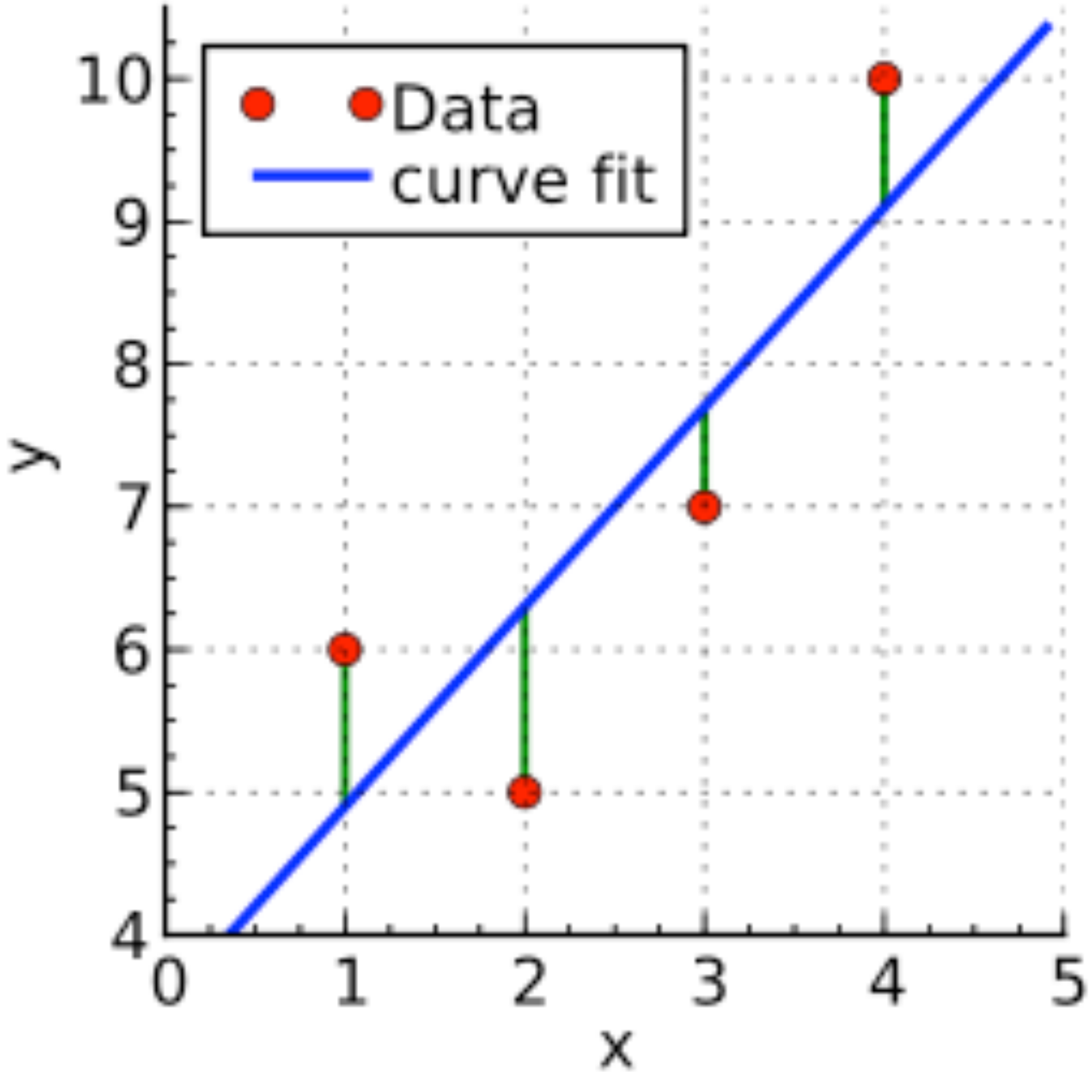
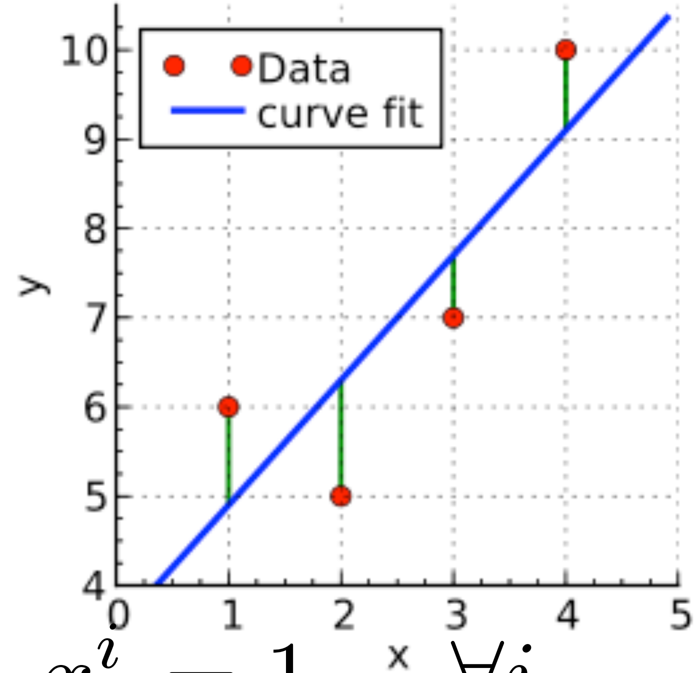
Linear regression in 1D



Linear regression in 1D



$$
\begin{aligned}
y^i &= w_0 + w_1 x_1^i + \epsilon^i \\
&= w_0 x_0^i + w_1 x_1^i + \epsilon^i, \quad x_0^i = 1, \ \forall i \\
&= \mathbf{w}^T \mathbf{x}^i + \epsilon^i
\end{aligned}
$$

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

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

Fitting a line

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

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

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

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

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

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

Fitting a line, continued

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

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

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

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

2 linear equations, 2 unknowns

Fitting a line, 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:

$$\left[\begin{array}{c} \sum_{i=1}^{N} y^i x_0^i \\ \sum_{i=1}^{N} y^i x_1^i \end{array} \right] = \left[\begin{array}{cc} \sum_{i=1}^{N} x_0^i x_0^i & \sum_{i=1}^{N} x_0^i x_1^i \\ \sum_{i=1}^{N} x_0^i x_1^i & \sum_{i=1}^{N} x_1^i x_1^i \end{array} \right] \left[\begin{array}{c} w_0 \\ w_1 \end{array} \right]$$

Fitting a line, continued

2x2 system of equations:

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

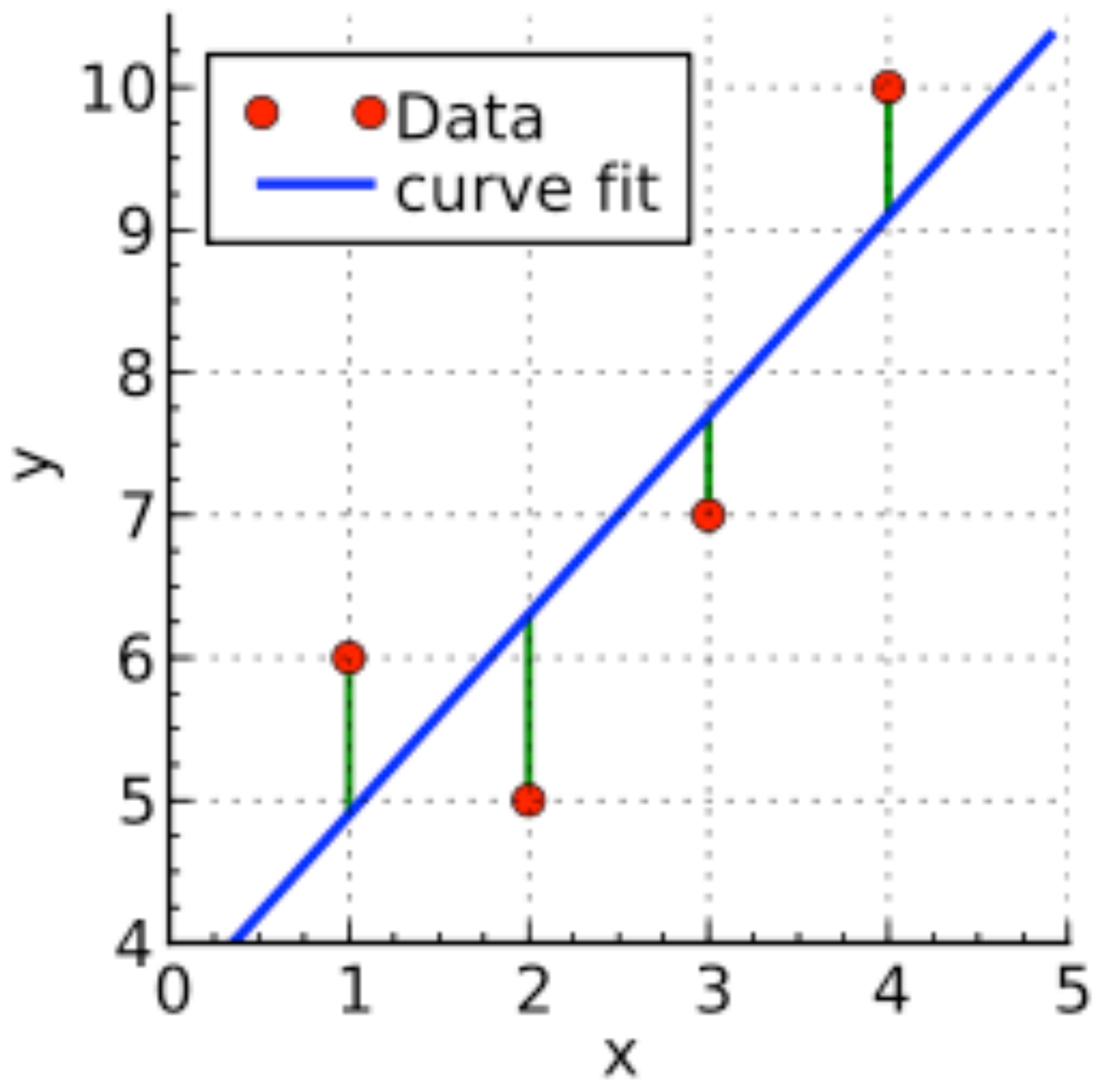
Or, without summations:

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

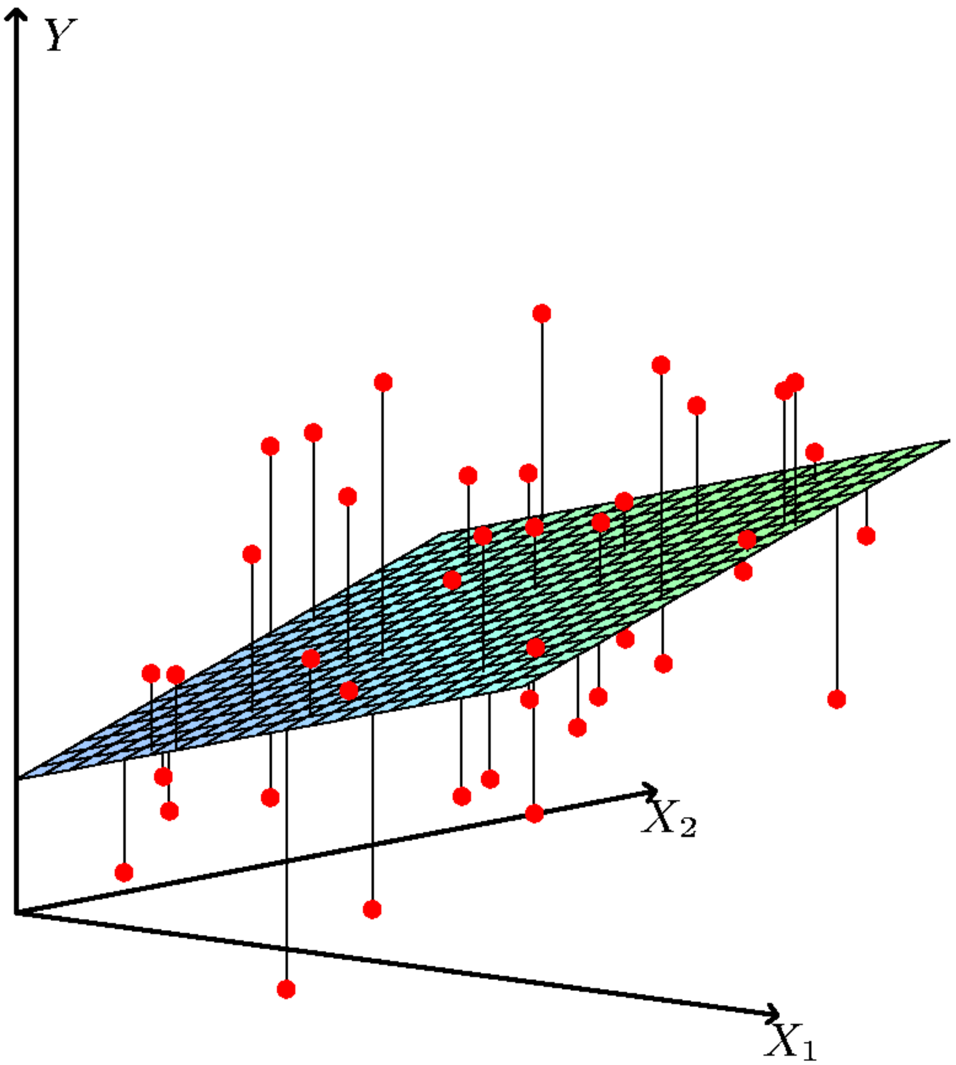
$$\mathbf{y} = \begin{bmatrix} y^1 \\ \vdots \\ y^N \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} x_0^1 & x_1^1 \\ \vdots & \vdots \\ x_0^N & x_2^N \end{bmatrix}$$

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

Linear regression in 1D



Linear regression in 2D (or ND)



What we would like to be happening

Training set: $S = \{(\mathbf{x}^i, y^i)\}, i = 1, \ldots, N$

$$y^1 = w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1$$

$$y^2 = w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2$$

$$\vdots$$

$$y^N = w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N$$

If N>D (e.g. 30 points, 2 dimensions) we have more equations than unknowns: **overdetermined** system!

Input-output relations can only hold approximately!

What is happening: approximations

Training set: $S = \{(\mathbf{x}^i, y^i)\}, i = 1, \ldots, N$

$$y^1 \simeq w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1$$

$$y^2 \simeq w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2$$

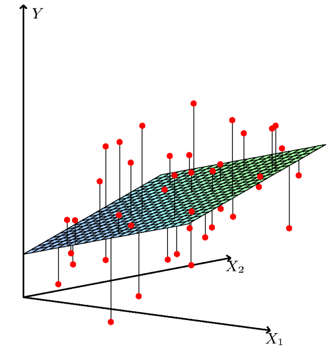
$$\vdots$$

$$y^N \simeq w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N$$

If N>D (e.g. 30 points, 2 dimensions) we have more equations than unknowns: **overdetermined** system!

Input-output relations can only hold approximately!

Goal: fit outputs with linear function



Training set: $S = \{(\mathbf{x}^i, y^i)\}, i = 1, \ldots, N$

$$y^1 = w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1 + \epsilon^1$$

$$y^2 = w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2 + \epsilon^2$$

$$\vdots$$

$$y^N = w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N + \epsilon^N$$

Objective: minimize sum of squared residuals

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

Least squares solution for linear regression

$$
\begin{aligned}
y^1 &= w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1 + \epsilon^1 \\
y^2 &= w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2 + \epsilon^2 \\
&\vdots \\
y^N &= w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N + \epsilon^N
\end{aligned}
$$

Least squares solution for linear regression

$$\begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^N \end{bmatrix} = \begin{bmatrix} x_0^1 & x_1^1 & \dots & x_D^1 \\ x_0^2 & x_2^2 & \dots & x_D^2 \\ \vdots & & & \\ x_0^N & x_2^N & \dots & x_D^N \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix} + \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

Nx1 **Nx(D+1)** **(D+1)x1** **Nx1**

Least squares solution for linear regression

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

Least squares solution for linear regression

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

$$L(\mathbf{w}) = \left[\begin{array}{cccc} \epsilon^1 & \epsilon^2 & \dots & \epsilon^N \end{array}\right] \left[\begin{array}{c} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{array}\right]$$

Least squares solution for linear regression

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

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

Least squares solution for linear regression

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

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

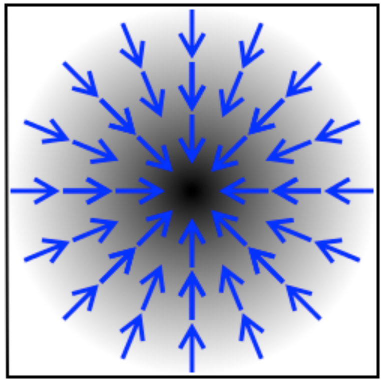
$$\begin{aligned} L(\mathbf{w}) &= \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} \\ &= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\mathbf{w} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w} \end{aligned}$$

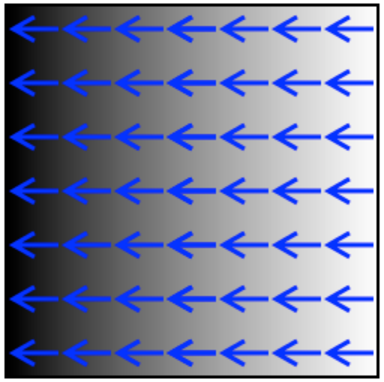
Gradient reminder

multivariate function: $f(x_1, \ldots, x_N)$

gradient:
$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_N} \end{bmatrix}$$

at extremum: $\nabla f = \mathbf{0}$





Minimizing the sum of squared errors in D-dimensions

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

Condition for minimum:

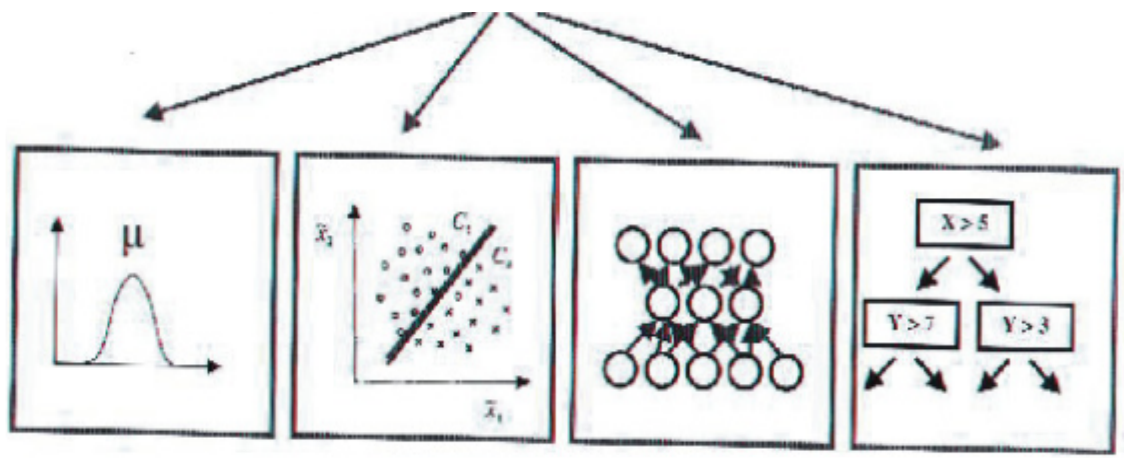
$$\nabla L(\mathbf{w}^*) = \mathbf{0}$$

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

Classifier function

- Input-output mapping
  - Output: y
  - Input: x
  - Method: f
  - Parameters: w

$$y = f_w(x) \quad (= f(x, w))$$



- Aspects of the learning problem
  - Identify methods that fit the problem setting
  - Determine parameters that properly classify the training set
  - Measure and control the `complexity' of these functions

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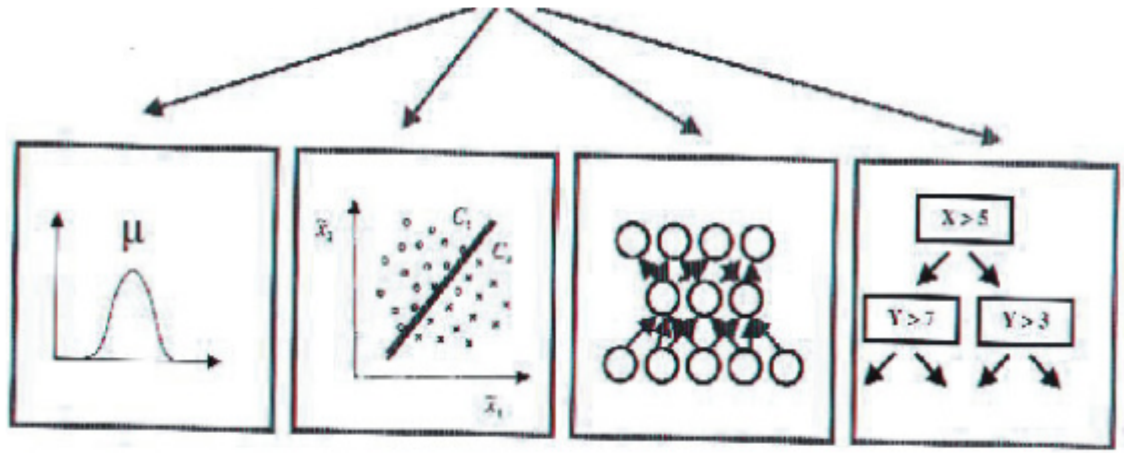

- Aspects of the learning problem
  - Identify methods that fit the problem setting
  - Determine parameters that properly classify the training set
  - Measure and control the `complexity’ of these functions

Done, for this method, and this notion of ‘proper’

Questions

Is the loss function appropriate for classification?

Quadratic loss: convex cost, closed-form solution

But does the optimized quantity indicate classifier's performance?

Is the classifier appropriate?

Linear classifier: fast computation

But could e.g. a non-linear classifier have better performance?

Are the estimated parameters good?

Parameters recover input-output mapping on training data

How can we know they do not simply memorize training data?

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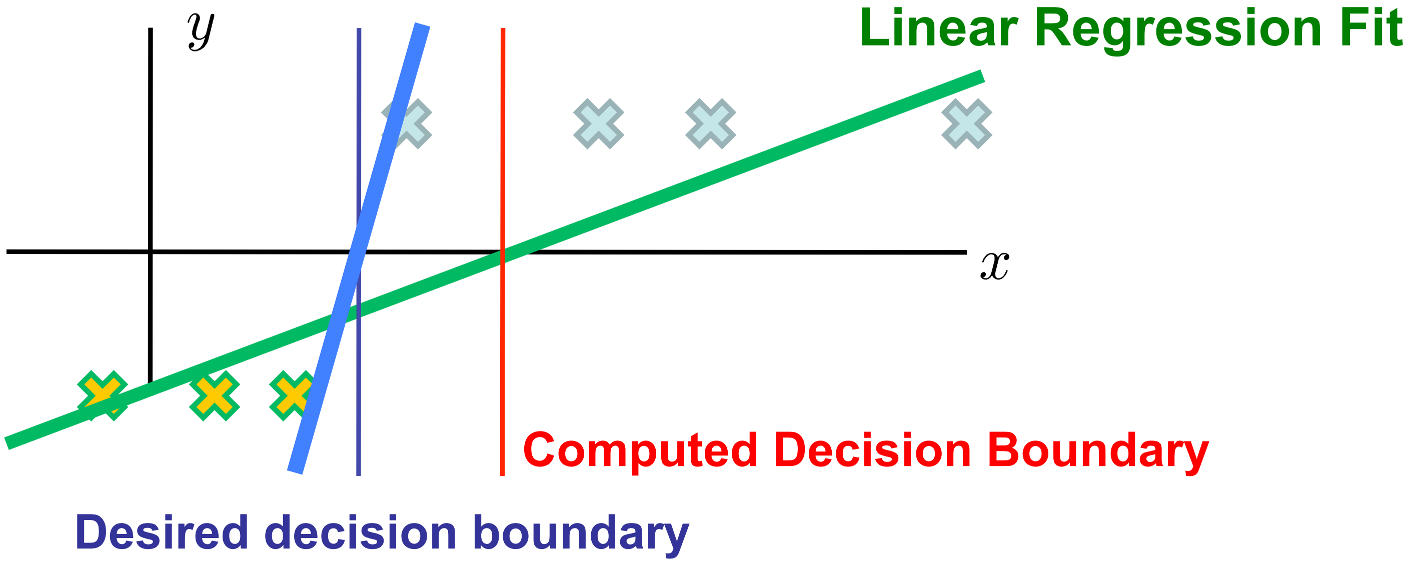
Inappropriateness of quadratic penalty

We chose the quadratic cost function for convenience

Single, global minimum & closed form expression

But does it indicate classification performance?

'Bad fit' according to our loss



Quadratic norm penalizes outputs that are `too good'

Logistic regression, SVMs, Adaboost: more appropriate loss

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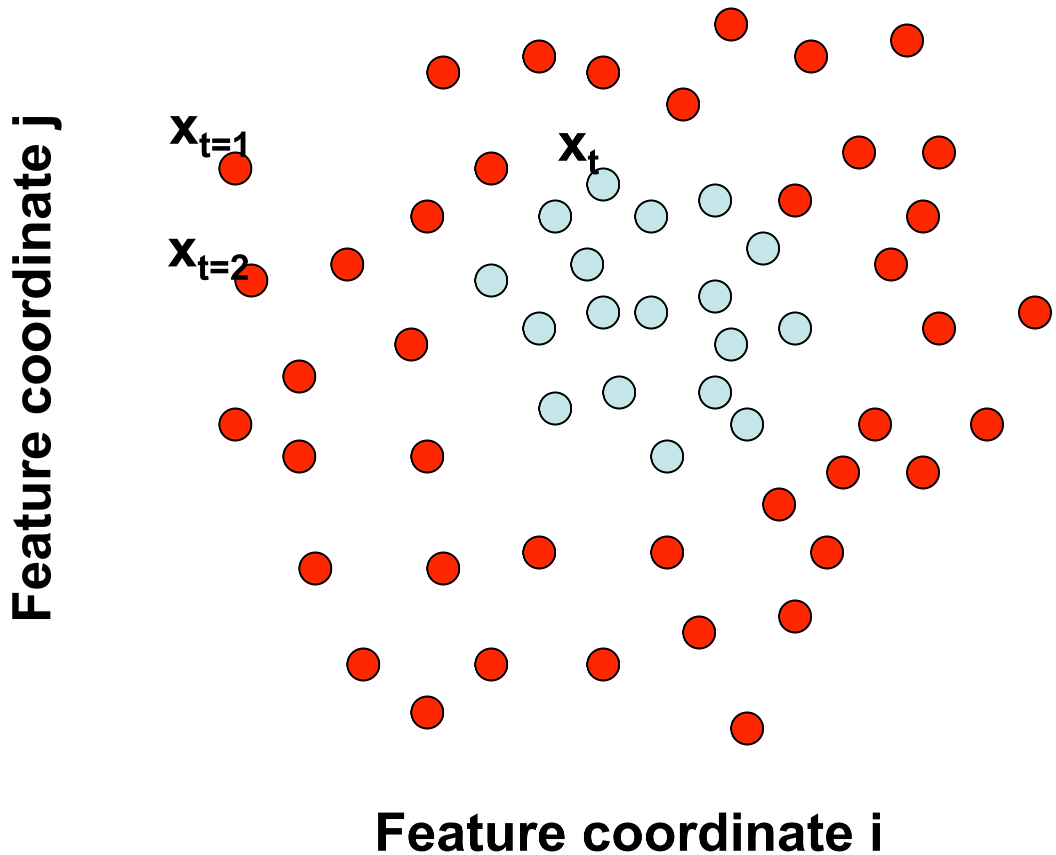
How can we know they do not simply memorize training data?

Classes may not be linearly separable

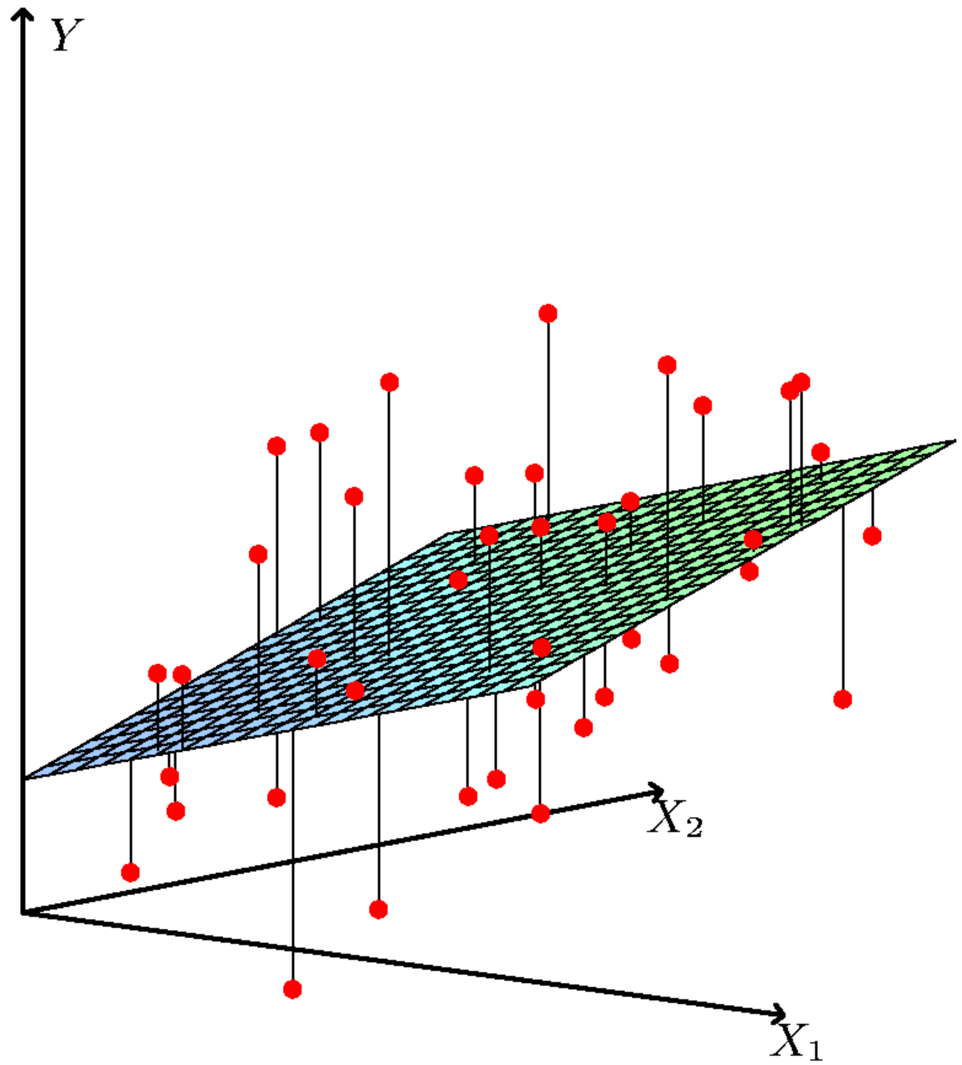
Linear function cannot properly separate these data



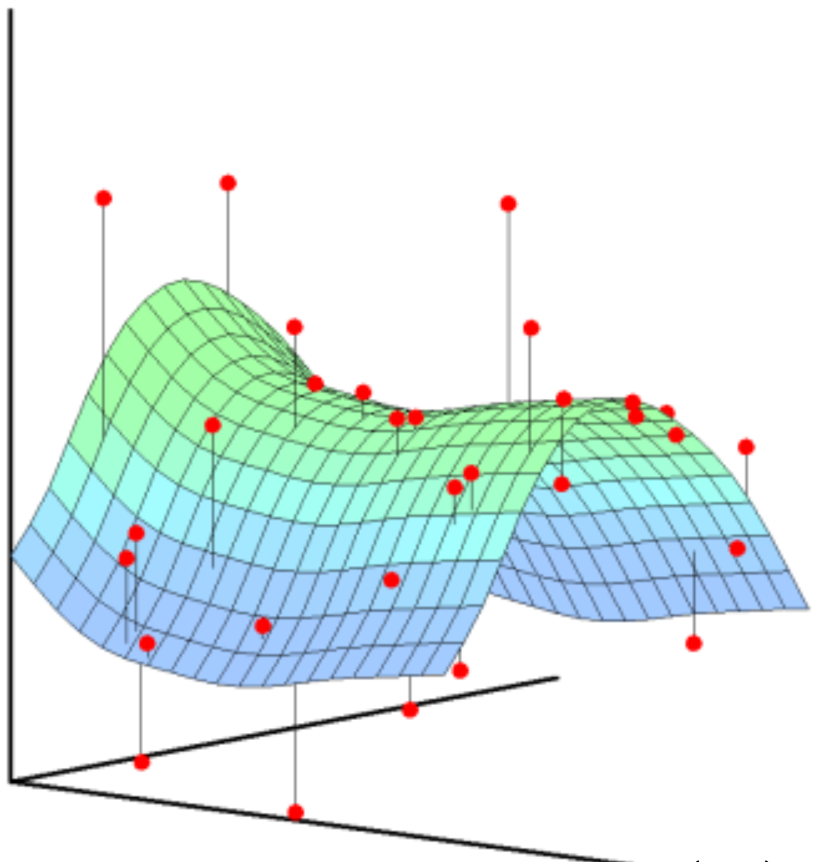
Each data point has a class label:

$$y_t = \begin{cases} +1 \; (\;) \\ -1 \; (\;) \end{cases}$$

Linear regression in 2D



Generalized linear regression



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

Example: second-order polynomials

$$\mathbf{x} = (x_1, x_2)$$

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ (x_1)^2 \\ (x_2)^2 \\ x_1 x_2 \end{bmatrix}$$

$$\langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}) \rangle = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2 + w_5 x_1 x_2$$

Reminder: linear regression

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

$$
\begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^N \end{bmatrix} = \begin{bmatrix} x_0^1 & x_1^1 & \dots & x_D^1 \\ x_0^2 & x_2^2 & \dots & x_D^2 \\ \vdots & & & \\ x_0^N & x_2^N & \dots & x_D^N \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix} + \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}
$$

Reminder: linear regression

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

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

generalized linear regression

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

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

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

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

Least squares solution for generalized linear regression

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

$$\mathbf{\Phi} = \left[\begin{array}{c} \phi(\mathbf{x}^1)^T \\ \hline \phi(\mathbf{x}^2)^T \\ \hline \vdots \\ \hline \phi(\mathbf{x}^N)^T \end{array}\right]$$

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

Minimize (as before):

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

Questions

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$$\langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}) \rangle = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2 + w_5 x_1 x_2$$

Example: fourth-order polynomials in 5 dimensions

$$\mathbf{x} = (x_1, \ldots, x_5)$$

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_5 \\ \vdots \\ (x_1 x_2 x_3 x_4 x_5)^4 \end{bmatrix}$$

15625 Dimensions =>15625 parameters

What was happening before: approximations

Training: $S = \{(\mathbf{x}^i, y^i)\}, i =, 1, \ldots, N$

$$y^1 \simeq w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1$$

$$y^2 \simeq w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2$$

$$\vdots$$

$$y^N \simeq w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N$$

If N>D (e.g. 30 points, 2 dimensions) we have more equations than unknowns: **overdetermined** system!

Input-output relations can only hold approximately!

What is happening now: overfitting

Training: $S = \{(\mathbf{x}^i, y^i)\}, i =, 1, \ldots, N$

$$y^1 = w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1$$

$$y^2 = w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2$$

$$\vdots$$

$$y^N = w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N$$

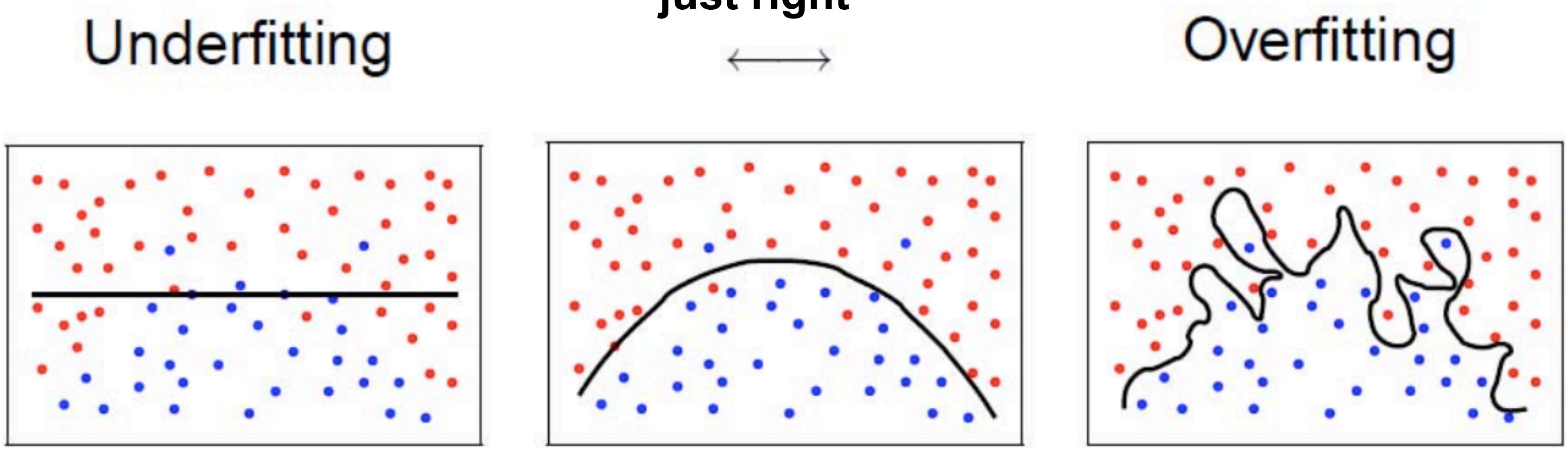
If N<D (e.g. 30 points, 15265 dimensions) we have more unknowns than equations: **underdetermined** system!

Input-output equations hold exactly, but we are simply memorizing data

Overfitting, in images

Classification

just right



Regression