Beyond Linear Regression

CS4061 / CS5014 Machine Learning

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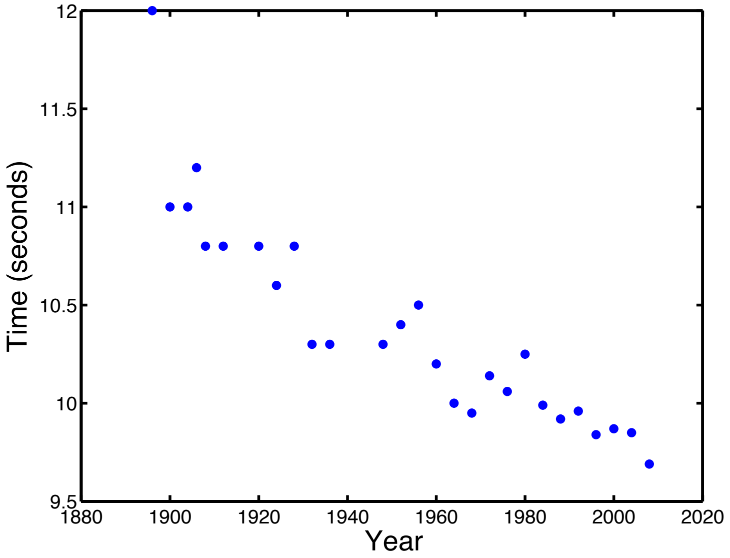
Time (seconds)
12
11.5
11
10.5
10
9.5
1880
1900
1920
1940
1960
1980
2000
2020
Year

What we did...

- wrote x for year and t for winning time
- training data: pairs $(x_1, t_1), (x_2, t_2), \ldots, (x_N, t_N)$

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- wrote x for year and t for winning time
- training data: pairs $(x_1,\ t_1),\ (x_2,\ t_2),\ \ldots,\ (x_N,\ t_N)$
- assumed some relationship: $t = f(x)$
- decided it's linear: $t = w_0 + w_1 x$

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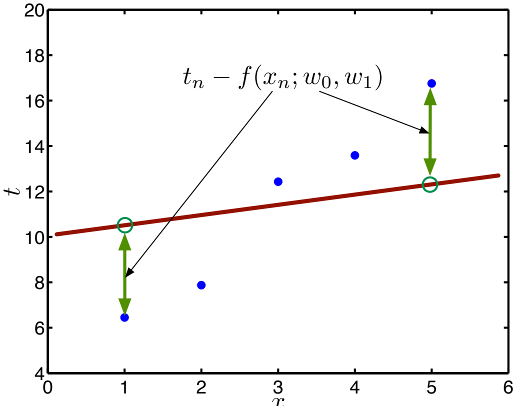
$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2$$



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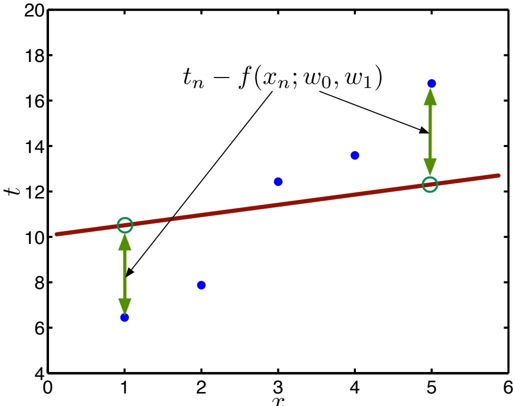
- characterised that mathematically:

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2 = \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2$$



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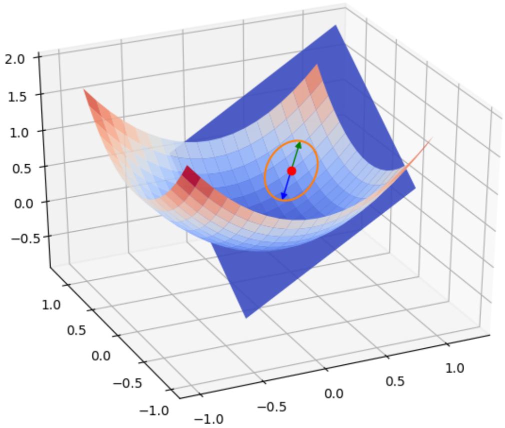

Figure: Pierre Vigier

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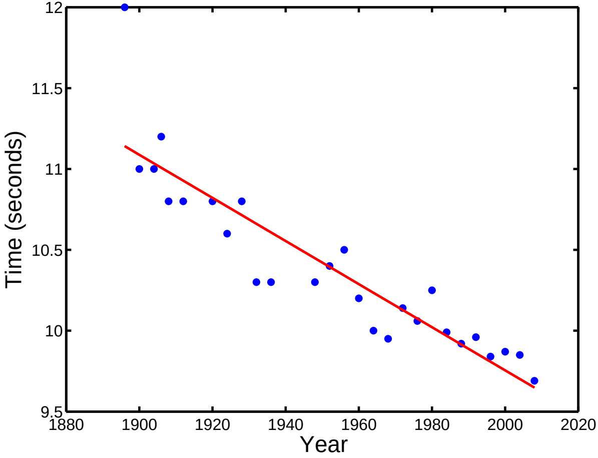
animation from https://pvigier.github.io/media/img/part1/gradient_descent.gif

Figure: Pierre Vigier



$$t = f(x) = 36.416 - 0.0133x$$

$$t_{2012} = f(2012) = 36.416 - 0.0133 \times 2012$$

$$t_{2012} = 9.59\ s$$

Assumptions

1. There exists a relationship between Olympic year and winning time
2. This relationship is linear (i.e. a straight line)
3. This relationship will continue into the future

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The model is ‘wrong’ but it might still be useful! How useful depends on the questions we wish to answer

What's next?

- Linear model in vector form
- Not-so-linear regression
- Generalisation, overfitting, cross-validation

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- We'll use bold, lowercase letters for vectors
- A list of values – similar to arrays when programming.

Vector model

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Vector model

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$$t = w_0 + w_1 x = \sum_{k=0}^{K} w_k x^k$$

Vector model

- Our model:

$$t = w_0 + w_1 x = \sum_{k=0}^{K} w_k x^k = \mathbf{w}^\mathsf{T}\mathbf{x}$$

- where...

$$\mathbf{w} = \left[\begin{array}{c} w_0 \\ w_1 \end{array}\right]$$

$$\mathbf{x} = \left[\begin{array}{c} x^0 \\ x^1 \end{array}\right] = \left[\begin{array}{c} 1 \\ x \end{array}\right]$$

- Vector model:

$$t = \mathbf{w}^\mathsf{T}\mathbf{x}$$

- Loss for n^{th} observation:

$$\mathcal{L}_n = (t_n - \mathbf{w}^\mathsf{T}\mathbf{x}_n)^2$$

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- Can we vectorize this further? Recall:

$$\sum_{d=1}^{D} a_d^2 = \mathbf{a}^\mathsf{T}\mathbf{a}$$

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$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N} q_n^2 = \frac{1}{N}\mathbf{q}^\mathsf{T}\mathbf{q} \quad \text{with} \;\; q_n = (t_n - \mathbf{w}^\mathsf{T}\mathbf{x}_n)$$

What is q?

$$q_n = (t_n - \mathbf{w}^\mathsf{T}\mathbf{x}_n)$$

...so...

$$\mathbf{q} = \begin{bmatrix} t_1 - \mathbf{w}^\mathsf{T}\mathbf{x}_1 \\ t_2 - \mathbf{w}^\mathsf{T}\mathbf{x}_2 \\ t_3 - \mathbf{w}^\mathsf{T}\mathbf{x}_3 \\ \vdots \\ t_N - \mathbf{w}^\mathsf{T}\mathbf{x}_N \end{bmatrix}$$

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Reminder: Subtracting vectors

$$\mathbf{a} - \mathbf{b} = \begin{bmatrix} a_1 - b_1 \\ a_2 - b_2 \\ \vdots \\ a_D - b_D \end{bmatrix}$$

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Matrices

- Stack all $\mathbf{x}_n^\top$ on top of one another:

$$\begin{matrix} [1, & x_1] \\ [1, & x_2] \\ \vdots & \\ [1, & x_N] \end{matrix}$$

Matrices

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$$\mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_N \end{bmatrix}$$

- This is a matrix
- We'll use bold, uppercase letters for matrices

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And the mean loss is:

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...still equiv. to

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)^2$$

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- Put data and parameters into vectors
- Written our model in vector form
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$$t = \mathbf{w}^\mathsf{T}\mathbf{x}, \quad \mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^\mathsf{T}(\mathbf{t} - \mathbf{X}\mathbf{w})$$

Different models, same loss

- We have a single loss that corresponds to many different models, with different $\mathbf{w}$ and $\mathbf{X}$

$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^{\mathsf{T}}(\mathbf{t} - \mathbf{X}\mathbf{w}).$$

- We can get an expression for the $\mathbf{w}$ that minimises $\mathcal{L}$, that will work for any of these models

Minimising the loss

- Given our vector/matrix loss

$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^\mathsf{T}(\mathbf{t} - \mathbf{X}\mathbf{w}),$$

- can take partial derivatives wrt vector $\mathbf{w}$ and set to zero:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \nabla_{\mathbf{w}}\mathcal{L} = \mathbf{0}$$

Minimising the loss

Summary

- Now we a have a general expression for best $\mathbf{w}$:

$$\widehat{\mathbf{w}} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t}$$

- Some examples...

Linear model – Olympic data

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}, \; \mathbf{X} = \begin{bmatrix} 1 & 1896 \\ 1 & 1900 \\ \vdots & \\ 1 & 2008 \end{bmatrix}, \; \mathbf{t} = \begin{bmatrix} 12.00 \\ 11.00 \\ \vdots \\ 9.85 \end{bmatrix}$$

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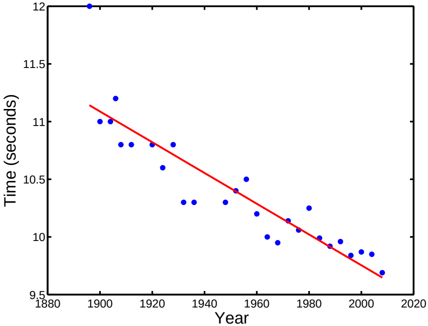
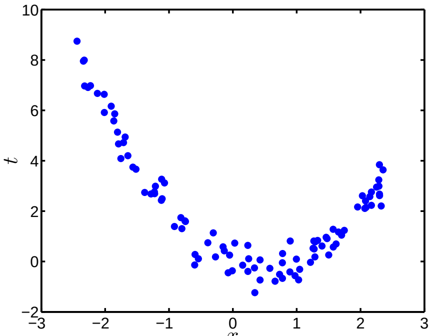


Quadratic model – synthetic data

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}, \ \mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 \end{bmatrix}$$



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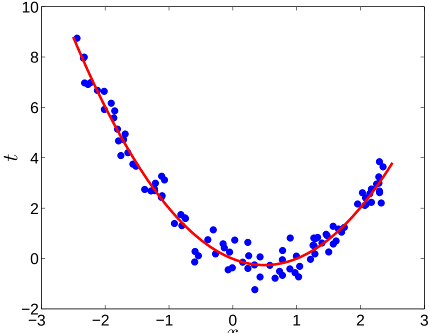
$$\widehat{\mathbf{w}} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t} = \begin{bmatrix} -0.0149 \\ -0.9987 \\ 1.0098 \end{bmatrix}$$

$$t_n = -0.0149 - 0.9987x_n + 1.0098x_n^2$$



8th order model – Olympic data

$$t = w_0 + w_1 x + w_2 x^2 + \ldots + w_8 x^8$$

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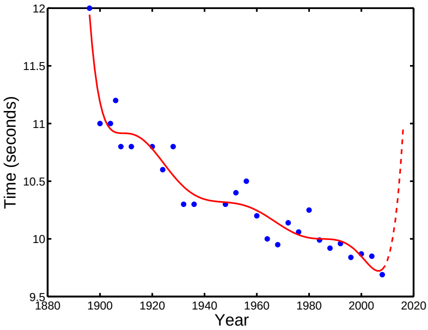

More general models

- So far, we've only considered functions of the form

$$t = w_0 + w_1 x + w_2 x^2 + \ldots + w_K x^K$$

- In fact, each term can be any function of x

$$t = w_0 h_0(x) + w_1 h_1(x) + \ldots + w_K h_K(x)$$

- For example,

$$t = w_0 + w_1 x + w_2 \sin(x) + w_3 x^{-1} + \ldots$$

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- In general:

$$\mathbf{X} = \begin{bmatrix} h_0(x_1) & h_1(x_1) & \ldots & h_K(x_1) \\ h_0(x_2) & h_1(x_2) & \ldots & h_K(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ h_0(x_N) & h_1(x_N) & \ldots & h_K(x_N) \end{bmatrix}$$

Example – Olympic data

$$t = w_0 + w_1 x + w_2 \sin\left(\frac{x-a}{b}\right)$$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}, \; \mathbf{X} = \begin{bmatrix} 1 & x_1 & \sin((x_1 - a)/b) \\ \vdots & \vdots & \vdots \\ 1 & x_N & sin((x_N - a)/b) \end{bmatrix}$$

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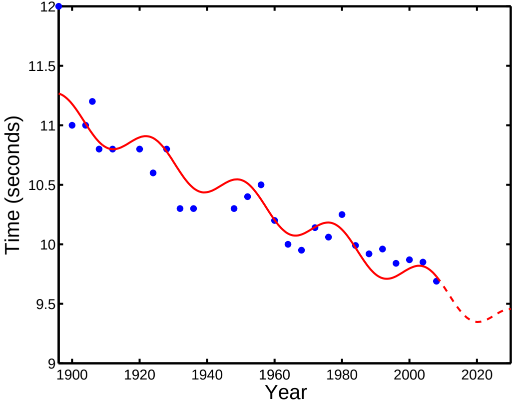
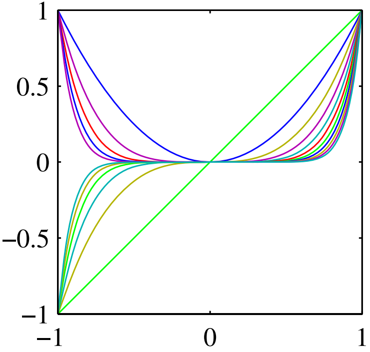


Common basis functions $h(x)$

Polynomial

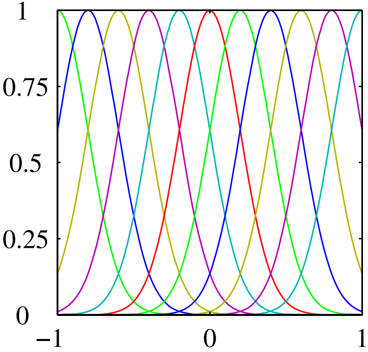
$$h_k(x) = x^k$$



Common basis functions $h(x)$

Radial basis function (RBF)

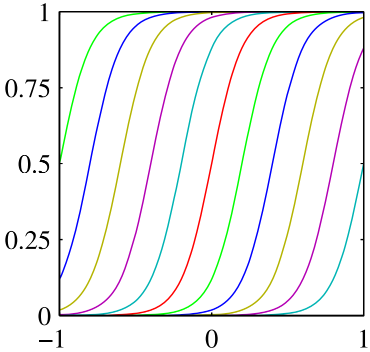
$$h_k(x) = \exp\left(-\frac{(x - \mu_k)^2}{2s^2}\right)$$



Common basis functions $h(x)$

Sigmoid

$$h_k(x) = \sigma\left(\frac{(x-\mu_k)^2}{s}\right)$$
$$\sigma(a) = \frac{1}{1+\exp(-a)}$$



Making predictions

$$\widehat{\mathbf{w}} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{t}$$

Where $\mathbf{X}$ depends on the choice of model:

$$\mathbf{X} = \begin{bmatrix} h_0(x_1) & h_1(x_1) & \dots & h_K(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ h_0(x_N) & h_1(x_N) & \dots & h_K(x_N) \end{bmatrix}$$

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To predict t at a new value of x, we first create $\mathbf{x}_{\text{new}}$:

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$$\mathbf{x}_{\mathrm{new}} = \begin{bmatrix} h_0(x_{\mathrm{new}}) \\ \vdots \\ h_K(x_{\mathrm{new}}) \end{bmatrix},$$

and then compute

$$t_{\mathrm{new}} = \widehat{\mathbf{w}}^\mathsf{T}\mathbf{x}_{\mathrm{new}}$$

Summary

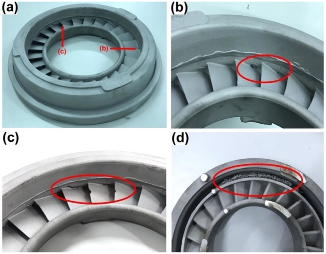
- Formulated our loss in terms of vectors and matrices
- Solved for best $\mathbf{w}$ (minimising the loss)
- Saw examples of models with differing numbers of terms
- Introduced basis functions

High-dimensional data

- input: image / audio / time-series / etc.

-   $\rightarrow$ **age**

High-dimensional data

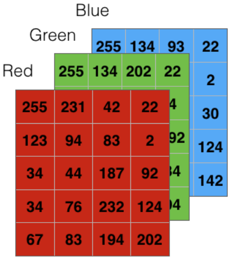
- input: image / audio / time-series / etc.
-  → **age**
- 

→ **defect severity**

Images: Karras, NeurIPS 2021; Huang, IJAMT 2019

Images

- Flatten images to vectors:



$$\begin{pmatrix} 255 \\ 231 \\ 42 \\ 22 \\ 123 \\ 94 \\ \vdots \\ \vdots \\ 92 \\ 142 \end{pmatrix} = \mathbf{x}_n$$

Photo: L Benoist; Diagram: S Dixon

Images

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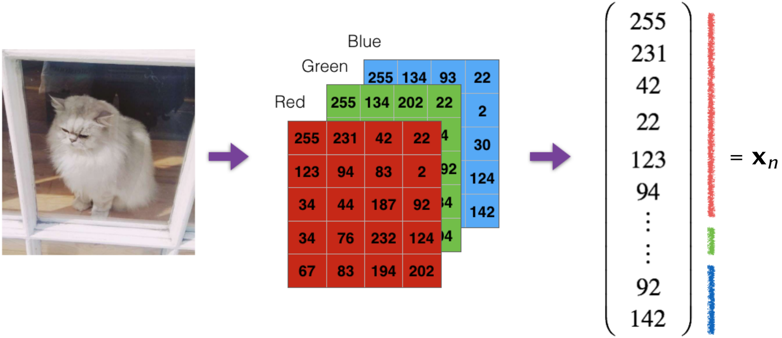

- $\mathbf{x}_n$ has millions of elements!

Photo: L Benoist; Diagram: S Dixon

High-dimensional data

1. **normalise / standardise**
   - centre faces in image
   - subtract average intensity; divide by standard deviation

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High-dimensional data

1. normalise / standardise
   - centre faces in image
   - subtract average intensity; divide by standard deviation
2. remove redundancy
   - subsample
   - convert to greyscale / simpler representation
3. **extract features**
   - landmark locations
   - blob attributes
   - *much lower-dimensional than pixels!*

Feature scaling

- attributes/features may differ in scale:

$$\mathbf{X} = \begin{pmatrix} 1 & 1896 & 21 \\ 1 & 1900 & 25 \\ \vdots & \vdots & \vdots \\ 1 & 2008 & 23 \end{pmatrix}$$

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$$\mathbf{X} = \begin{pmatrix} 1 & 1896 & 21 \\ 1 & 1900 & 25 \\ \vdots & \vdots & \vdots \\ 1 & 2008 & 23 \end{pmatrix}$$

- subtract mean
- divide by standard deviation

$$\mathbf{X} = \begin{pmatrix} 1 & -1.6 & -0.1 \\ 1 & -1.5 & 0.7 \\ \vdots & \vdots & \vdots \\ 1 & 1.6 & 0.3 \end{pmatrix}$$