AI4ER 0: Regression

Rich Turner
(with thanks to Miguel Hernandez Lobato for the slides)

What is regression?

A **type of problem** in machine learning requiring

- to identify **patterns** and **regularities** between **input variables** and a corresponding continuous **output variable**,
- from a **training data set** $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$ formed by pairs of input vectors $\mathbf{x}_n = (x_{n,1}, \ldots, x_{n,D})^\mathsf{T}$ and corresponding output values $y_n \in \mathbb{R}$.

Linear regression model

The relationship between inputs $\mathbf{x}_n$ and outputs y_n in $p(y_n|\mathbf{x}_n, \boldsymbol{\theta})$ is **linear**.

Why linear? Simple, easy to understand, widely used, easily generalized.

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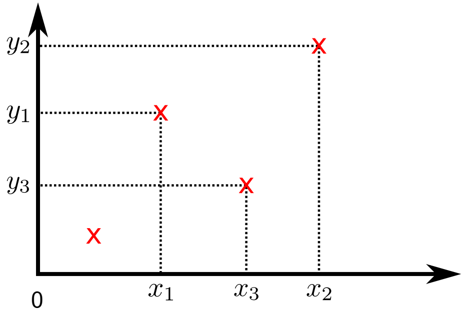

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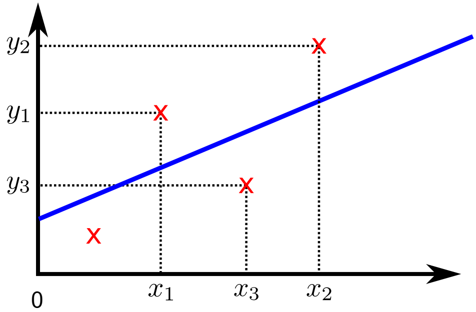

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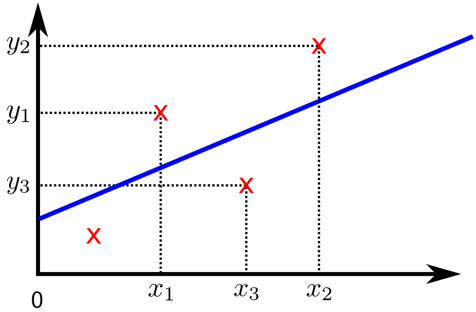

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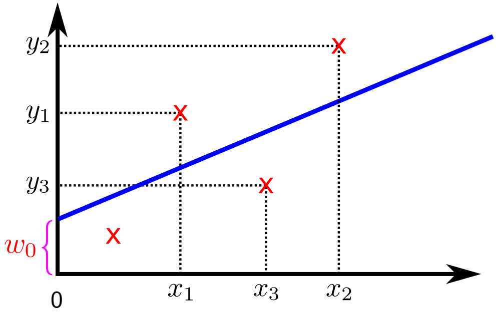

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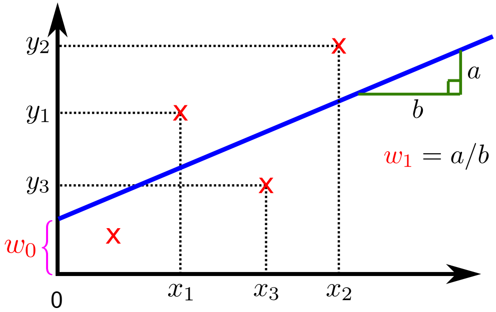

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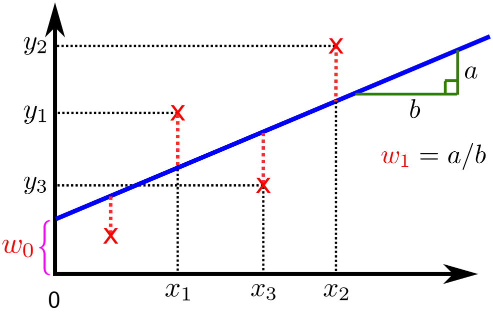

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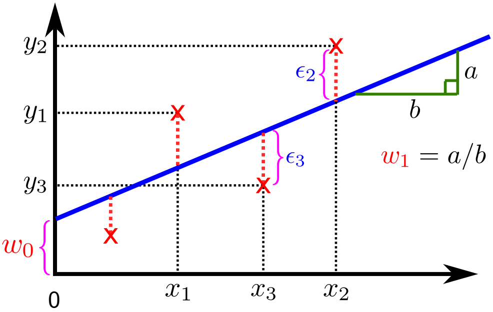

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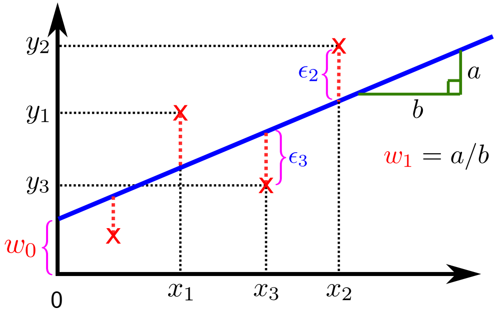

$$y_n = w_0 + w_1 x_n + \epsilon_n$$

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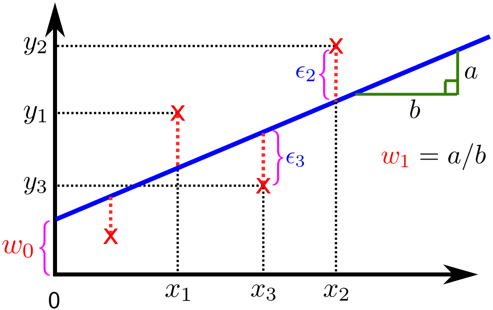

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What should the distribution of ϵ_n be?

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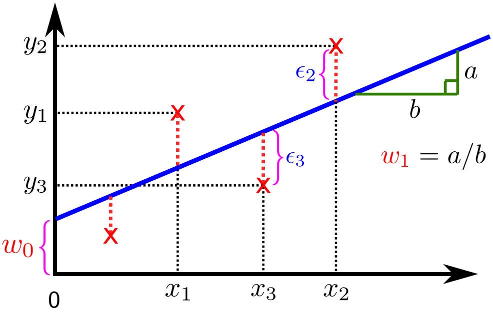

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What should the distribution of ϵ_n be?

$\epsilon_n \sim \mathcal{N}(0, \sigma^2)$ allows for tractable inference.

Linear regression model

Assuming

$$y_n = w_0 + w_1 x_n + \epsilon_n \,,$$

$$\epsilon_n \sim \mathcal{N}(0, \sigma^2)\,.$$

What is the form of $p(y_n|\mathbf{x}_n, \boldsymbol{\theta})$ with $\boldsymbol{\theta} = \{\sigma^2, w_0, w_1\}$?

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We have that

$$\mathbf{E}[y_n] = w_0 + w_1 x_n + \mathbf{E}[\epsilon_n] = w_0 + w_1 x_n \,,$$
$$\mathrm{Var}[y_n] = \mathbf{E}\left[(y_n - \mathbf{E}[y_n])^2\right] = \mathbf{E}\left[{\epsilon_n}^2\right] = \sigma^2 \,.$$

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Therefore,

$$\begin{aligned} p(y_n | \mathbf{x}_n, \boldsymbol{\theta}) &= \mathcal{N}(y_n | w_0 + w_1 x_n, \sigma^2) \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{ -\frac{1}{2} \frac{(y_n - w_0 - w_1 x_n)^2}{\sigma^2} \right\} \,. \end{aligned}$$

Linear regression in higher dimensions

For a data set $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$, we assume

$$y_n = w_0 + w_1 x_{n,1} + \cdots + w_D x_{n,D} + \epsilon_n$$

where $\boxed{\epsilon_n \sim \mathcal{N}(0, \sigma^2)}$ and $\widetilde{\mathbf{x}}_n = (1, \mathbf{x}_n)^{\mathsf{T}}$, $\boldsymbol{\theta} = \{\sigma^2, \mathbf{w}\}$.

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Jargon for regression:

- $\mathbf{x}_n$ are the inputs, features, covariates, independent variables, etc.
- $\mathbf{y}_n$ are the outputs, responses, targets, dependent variables, etc.
- $\mathbf{w}$ are the coefficients, weights, etc. (w_0 is called the bias or intercept).
- ϵ_n are the errors, disturbances or noise.

Inference: Maximum Likelihood Estimate (MLE)

Maximize the **likelihood** function $p(y_1, \ldots, y_n | \widetilde{\mathbf{x}}_1, \ldots, \widetilde{\mathbf{x}}_n, \boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$.

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&= \sum_{n=1}^{N} \left\{ -\frac{1}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} (y_n - \mathbf{w}^{\mathsf{T}} \widetilde{\mathbf{x}}_n)^2 \right\}
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where $\mathbf{y} = (y_1, \ldots, y_n)^\mathsf{T}$, $\widetilde{\mathbf{X}} = (\widetilde{\mathbf{x}}_1; \ldots; \widetilde{\mathbf{x}}_n)^\mathsf{T}$, and we have used $\mathbf{a}^\mathsf{T} \mathbf{a} = \sum_i a_i^2$.

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&= -\frac{N}{2} \log(2\pi\sigma^2) - \frac{\mathbf{y}^\mathsf{T} \mathbf{y}}{2\sigma^2} - \underbrace{\frac{\mathbf{w}^\mathsf{T} \widetilde{\mathbf{X}}^\mathsf{T} \widetilde{\mathbf{X}} \mathbf{w}}{2\sigma^2}}_{\text{Quadratic term}} + \underbrace{\frac{\mathbf{y}^\mathsf{T} \widetilde{\mathbf{X}} \mathbf{w}}{\sigma^2}}_{\text{Linear term}} .
\end{aligned}$$

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Vector calculus I

$$\mathbf{a} = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_D \end{bmatrix}, \qquad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_D \end{bmatrix}, \qquad \mathbf{a}^\mathsf{T}\mathbf{w} = \sum_{i=0}^{D} a_i w_i \,,$$

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Vector calculus II

Using the previous result

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and the product rule of calculus,

$$\frac{d}{dx}[f(x)g(x)] = \underbrace{[\frac{d}{dx}f(x)]g(x)}_{g(x) \text{ as constant}} + \underbrace{f(x)[\frac{d}{dx}g(x)]}_{f(x) \text{ as constant}}\,, \tag{1}$$

we obtain

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Finding the maximum likelihood parameters

The gradient of the log-likelihood at the maximizer is zero.

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$$\sigma^2 = \frac{1}{N} \left(\mathbf{y} - \widetilde{\mathbf{X}} \mathbf{w} \right)^{\mathsf{T}} \left(\mathbf{y} - \widetilde{\mathbf{X}} \mathbf{w} \right) \,.$$

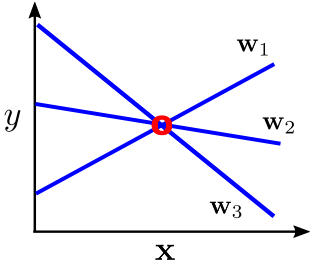
Problems of MLE

When $N < D + 1$ the MLE

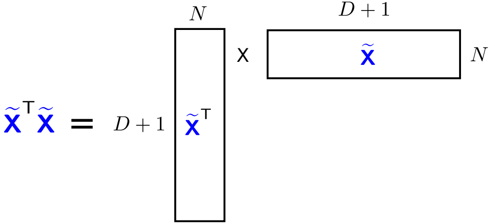
$$\mathbf{w} = \left(\widetilde{\mathbf{X}}^\mathsf{T}\widetilde{\mathbf{X}}\right)^{-1}\widetilde{\mathbf{X}}^\mathsf{T}\mathbf{y}$$

is not defined. In this case...

Many values of $\mathbf{w}$ fit the training data equally well, achieving **zero error**.



The matrix $\widetilde{\mathbf{X}}^\mathsf{T}\widetilde{\mathbf{X}}$ is low rank and not invertible:



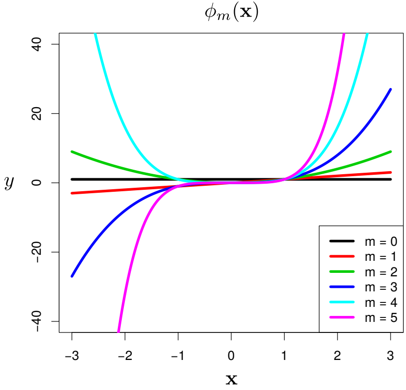
Non-linear (basis function) regression

Linear regression can model non-linear relationships by replacing $\mathbf{x}$ with some non-linear function of the inputs $\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \ldots, \phi_M(\mathbf{x}))^\mathsf{T}$.

Inference does not change, just replace each $\mathbf{x}_n$ with the new $\phi(\mathbf{x}_n)$.

Example, **polynomials** for 1D data $\phi_m(x) = x^m$, $m = 1, \ldots, M$:

$$
\begin{aligned}
M = 0\,, &\quad \phi(x) = [1]^\mathsf{T}\,,\\
M = 1\,, &\quad \phi(x) = [1, x]^\mathsf{T}\,,\\
M = 2\,, &\quad \phi(x) = [1, x, x^2]^\mathsf{T}\,,\\
M = 3\,, &\quad \phi(x) = [1, x, x^2, x^3]^\mathsf{T}\,,\\
M = 4\,, &\quad \phi(x) = [1, x, x^2, x^3, x^4]^\mathsf{T}\,,\\
M = 5\,, &\quad \phi(x) = [1, x, x^2, x^3, x^4, x^5]^\mathsf{T}\,,
\end{aligned}
$$



What should the value of M be?

1D example with polynomials

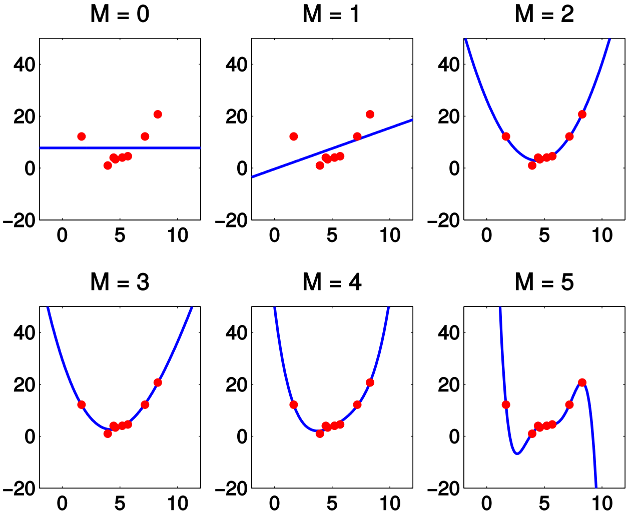
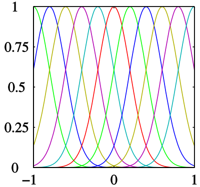


Figure: Z. Ghahramani.

Other basis functions

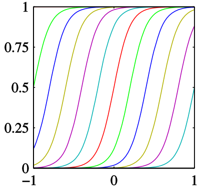
Gaussian radial basis functions with center $\mathbf{c}_m$ and width s:

$$\phi_m(\mathbf{x}) = \exp\left\{-\frac{1}{2}s(\mathbf{x},\mathbf{c}_m,s)^2\right\}$$
$$s(\mathbf{x},\mathbf{c}_m,s) = \sqrt{(\mathbf{x}-\mathbf{c}_m)^\mathsf{T}(\mathbf{x}-\mathbf{c}_m)/s^2}\,.$$



Sigmoidal basis functions:

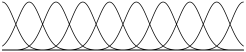
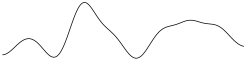
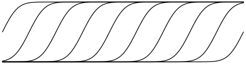
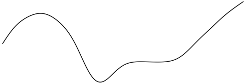
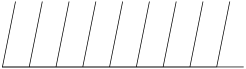
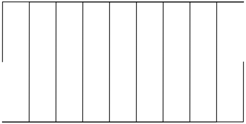
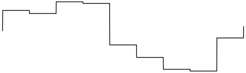
$$\phi_m(\mathbf{x}) = \sigma\left(s(\mathbf{x},\mathbf{c}_m,s)\right)$$
$$\sigma(x) = \frac{1}{1+\exp(-x)}\,.$$



They are uniformly spread in input space to capture non-linearities everywhere.

Figure: C. Bishop. *Pattern Recognition and Machine Learning*, 2006.

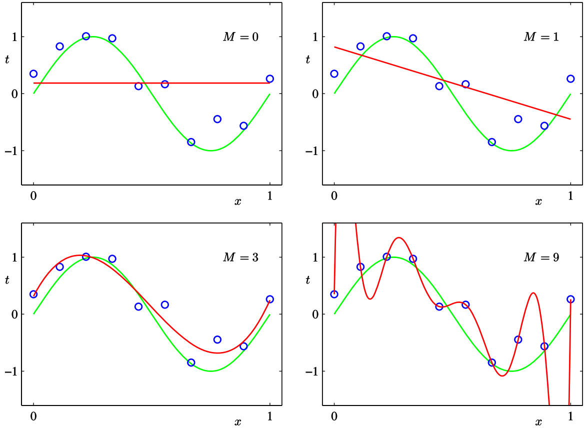
Examples

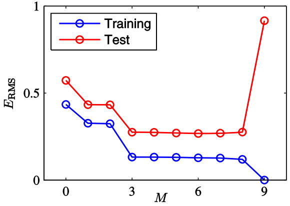
$\phi_m(\mathbf{x})$	Type of basis function	$\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x})$
$\mathcal{N}(x \mid c_m, 1)$	Gaussian 	
$\dfrac{1}{1+\exp(-x+c_m)}$	Sigmoidal 	
$\max(0, x-c_m)$	Truncated linear 	
$\mathrm{sign}(x-c_m)$	Step functions 	

$c_1 = -10$, $c_2 = -8$, $\ldots$, $c_9 = 8$, $c_{10} = 10$, $s = 1$.

Overfitting

A large number of basis functions can lead to **over-fitting**: the model fits the **training data** well but it performs poorly on new **test data**.





	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Solution: use a prior distribution to enforce the entries of $\mathbf{w}$ to be small.

Figures and table: C. Bishop. *Pattern Recognition and Machine Learning*, 2006.