TDA231
Linear Regression: Modelling the noise

Devdatt Dubhashi
dubhashi@chalmers.se

Dept. of Computer Science and Engg.
Chalmers University

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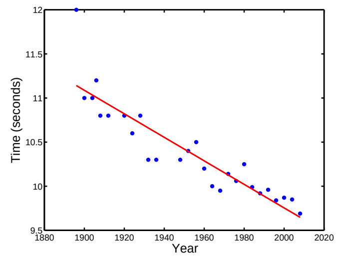
What about the errors?

$$t = w_0 + w_1 x = \mathbf{w}^\mathsf{T}\mathbf{x}$$

$$t = w_0 + w_1 x + w_2 x^2 + w_3 x^2 + \ldots + w_K x^K = \sum_{k=0}^{K} w_k x^k = \mathbf{w}^\mathsf{T}\mathbf{x}$$



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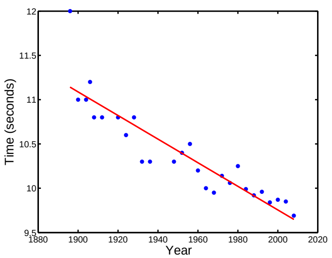
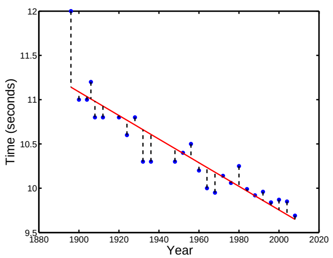
$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^\mathsf{T}\mathbf{x}_n\right)^2$$

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





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We **should** model the errors

- We know they're there - shouldn't ignore them.

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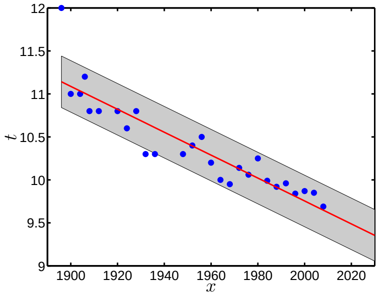

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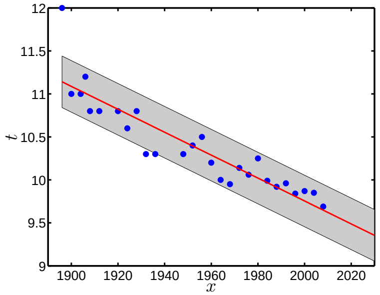

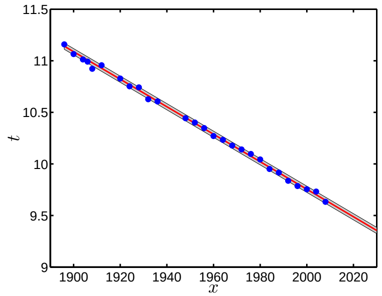

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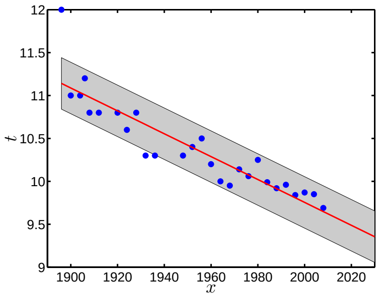
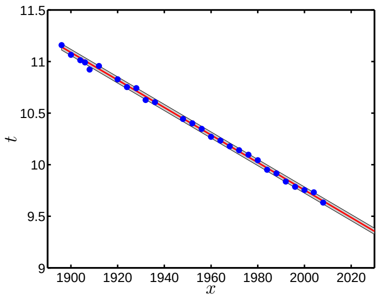
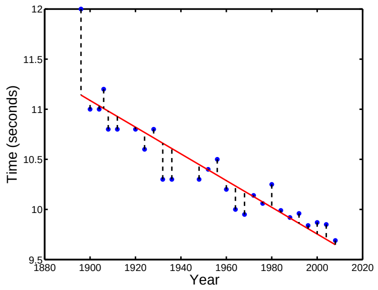




- ...and other reasons that we will get to later...

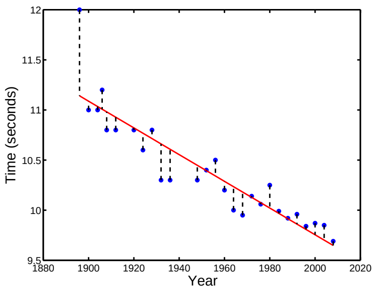
Additive errors



We'll assume that the noise is an additive term in the model:

$$t_n = \mathbf{w}^\mathsf{T}\mathbf{x} + \epsilon_n$$

Additive errors



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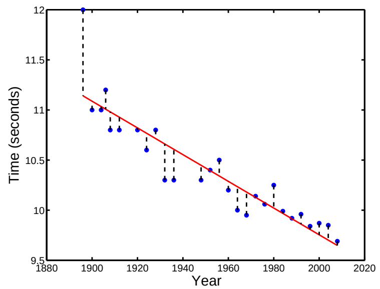

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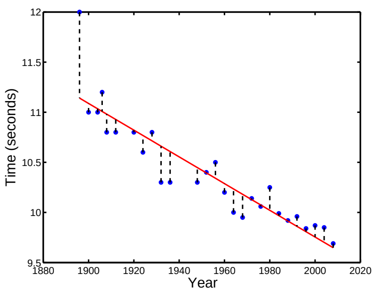
Additive errors



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- It's different for each n.
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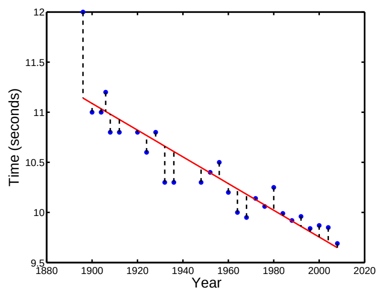

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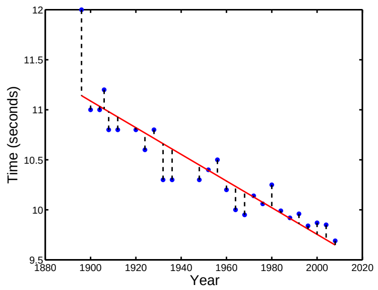

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What assumptions can we make about ϵ_n?

- It's different for each n.
- It's positive and negative.
- There doesn't seem to be any relationship between ϵ at different n.
- Looks very hard to model exactly (if it were, it wouldn't be noise!)

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Gaussian noise model

- Our model:

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- ϵ_n is continuous.
- We need to choose $p(\epsilon)$.

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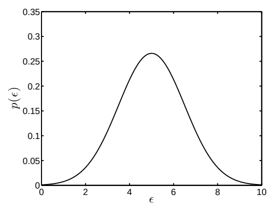
- Gaussian:



$$p(\epsilon|\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma^2}(\epsilon-\mu)^2\right\}$$

Gaussian noise model

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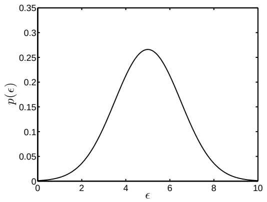
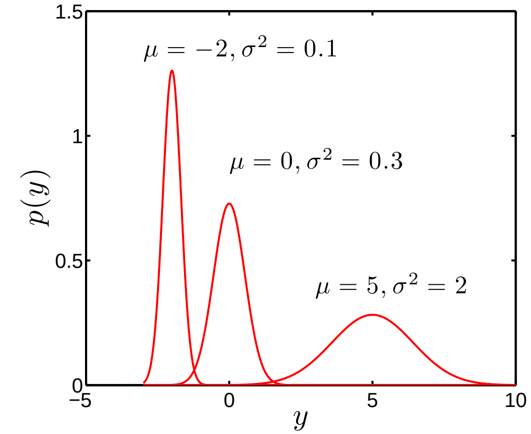


$$p(\epsilon|\mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma^2}(\epsilon - \mu)^2\right\}$$

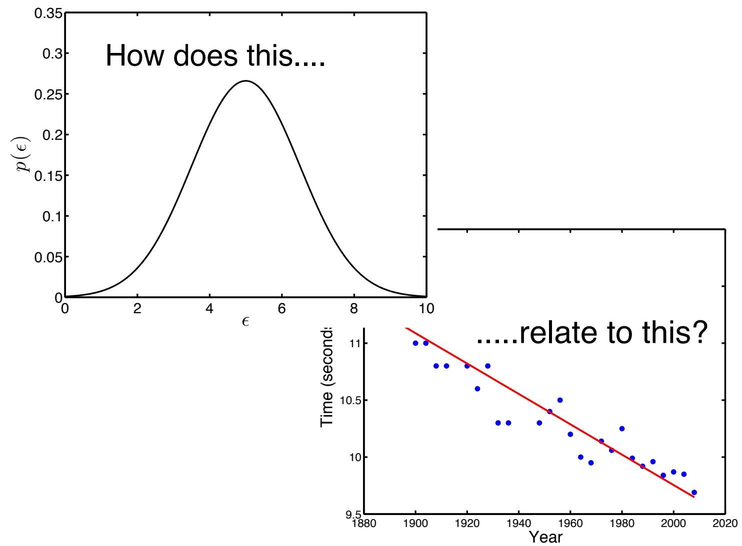
- 2 parameters: Mean μ and Variance σ^2.

Gaussian examples



Effect of varying the mean (μ) and variance (σ^2) parameters of the Gaussian.

Generating data



Likelihood

- Evaluate the density:

$$p(t|\mathbf{x}_n, \mathbf{w}, \sigma^2) = \mathcal{N}(\mathbf{w}^\mathsf{T}\mathbf{x}_n, \sigma^2)$$

- at $t = t_n$ is called for the Likelihood.

Likelihood

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- The higher the value, the more likely t_n is given the model....

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Likelihood

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- at $t = t_n$ is called for the Likelihood.
- The higher the value, the more likely t_n is given the model....
  - ....the better the model is.

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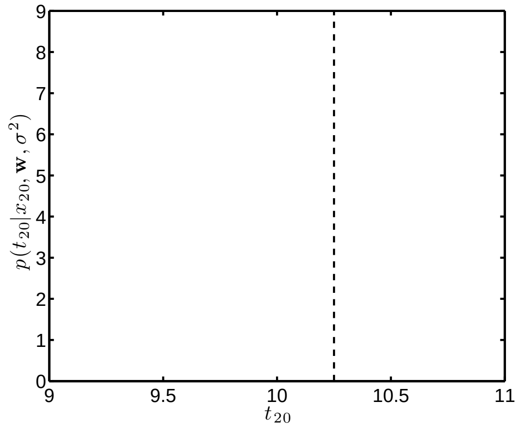

Lets look at the 1980 Olympics ($n = 20$).
Dashed line shows t_{20}.

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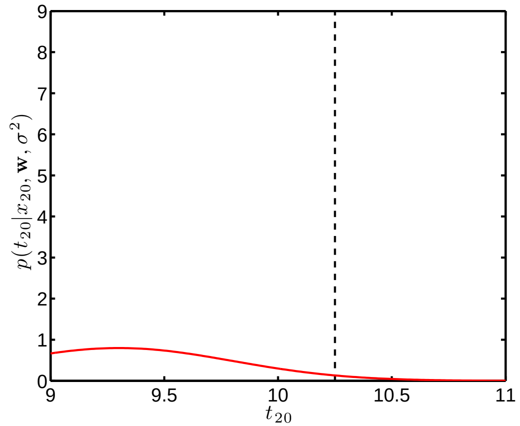
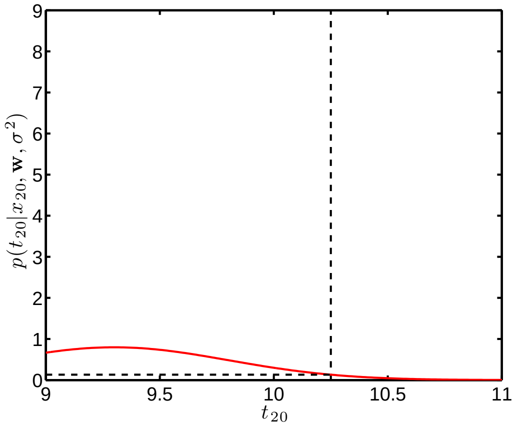
Likelihood



Model 1. Red line shows $\mathcal{N}(\mathbf{w}^\mathsf{T}\mathbf{x}_n, \sigma^2)$

Likelihood



$p(t_{20}|\dots) \approx 0.1.$

Likelihood

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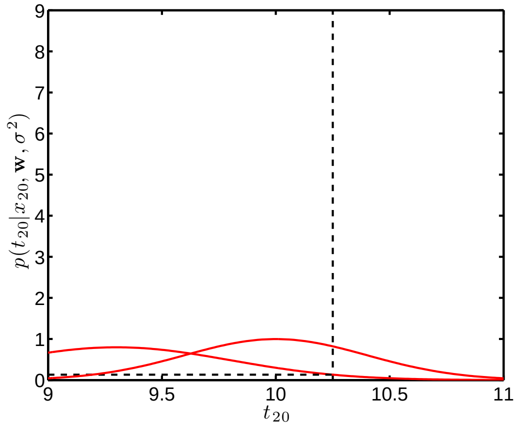

Model 2. Red line shows $\mathcal{N}(\mathbf{w}^\mathsf{T}\mathbf{x}_n, \sigma^2)$ for a different $\mathbf{w}$

Likelihood

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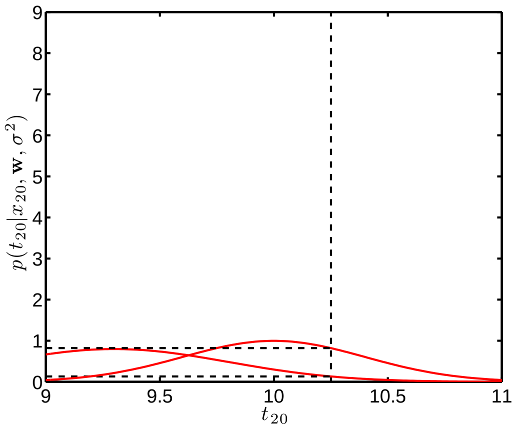

$p(t_{20}|\dots) \approx 0.9.$

Likelihood

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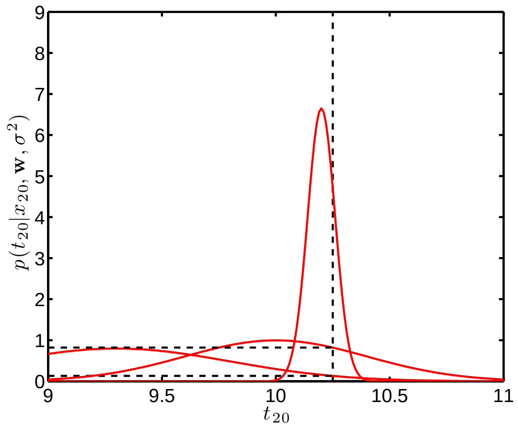
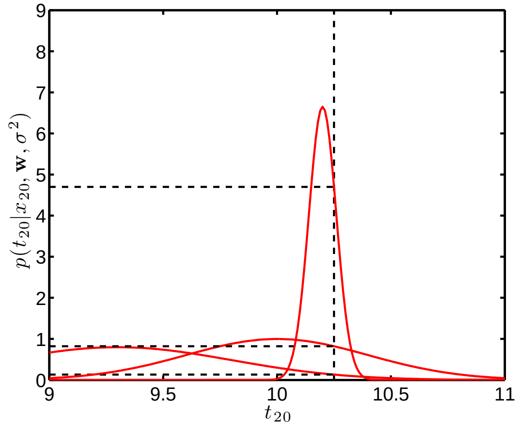


Model 3.

Likelihood



Model 3.

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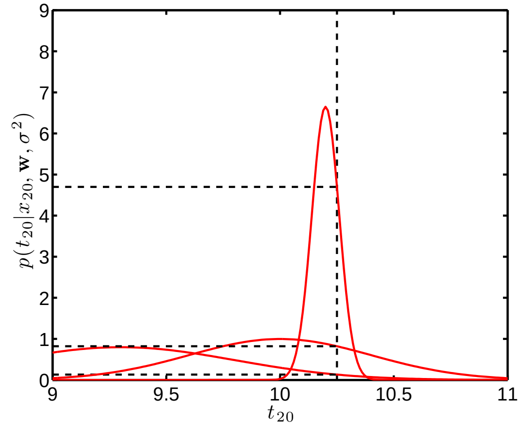
Likelihood



Model 3.

Model 3 looks best.

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Likelihood

- The value we get when we evaluate the density function is called the **likelihood**.

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Likelihood

- The value we get when we evaluate the density function is called the **likelihood**.
- i.e.
  - The likelihood for model 1 was 0.1.
  - The likelihood for model 2 was 0.9.
  - The likelihood for model 3 was 4.8.
- For continuous random variables, it is **not** a probability!

Likelihood

- The value we get when we evaluate the density function is called the **likelihood**.
- i.e.
  - The likelihood for model 1 was 0.1.
  - The likelihood for model 2 was 0.9.
  - The likelihood for model 3 was 4.8.
- For continuous random variables, it is **not** a probability!
- As t_n is fixed, we can find the values of $\mathbf{w}$ and σ^2 that maximise the likelihood.
  - ...just like we found them that minimised the loss.

Likelihood optimisation

- For each input-response pair, we have a Gaussian likelihood:

$$p(t_n|\mathbf{w}, \mathbf{x}_n, \sigma^2) = \mathcal{N}(\mathbf{w}^\mathsf{T}\mathbf{x}_n, \sigma^2)$$

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- To combine them all, we want the joint likelihood:

$$p(t_1, \ldots, t_N|\mathbf{w}, \sigma^2, \mathbf{x}_1, \ldots, \mathbf{x}_N)$$

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- To combine them all, we want the joint likelihood:

$$p(t_1, \ldots, t_N|\mathbf{w}, \sigma^2, \mathbf{x}_1, \ldots, \mathbf{x}_N)$$

- Assume that the t_n are independent:

$$p(t_1, \ldots, t_N|\mathbf{w}, \sigma^2, \mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{n=1}^{N} p(t_n|\mathbf{w}, \mathbf{x}_n, \sigma^2)$$

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Likelihood optimisation

Finding the parameters that maximise the likelihood is expressed mathematically as:

$$\underset{\mathbf{w},\sigma^2}{\text{argmax}} \prod_{n=1}^{N} p(t_n|\mathbf{w},\mathbf{x}_n,\sigma^2)$$

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In fact, we'll optimise the (natural) log likelihood because it's easier.

- If we increase z, $\log(z)$ increases, if we decrease z, $\log(z)$ decreases. So, at a maximum of z, $\log(z)$ will also be at a maximum.

Likelihood optimisation

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$$\underset{\mathbf{w},\sigma^2}{\text{argmax}} \log \prod_{n=1}^{N} p(t_n|\mathbf{w},\mathbf{x}_n,\sigma^2)$$

Some re-arranging...

$$\begin{aligned} p(t_n|\mathbf{w},\mathbf{x}_n,\sigma^2) &= \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma^2}(t_n - \mathbf{w}^\mathsf{T}\mathbf{x}_n)^2\right\} \\ \log L &= \log \prod_{n=1}^{N} p(t_n|\mathbf{w},\mathbf{x}_n,\sigma^2) \end{aligned}$$

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p(t_n|\mathbf{w},\mathbf{x}_n,\sigma^2) &= \frac{1}{\sigma\sqrt{2\pi}}\exp\left\{-\frac{1}{2\sigma^2}(t_n-\mathbf{w}^\mathsf{T}\mathbf{x}_n)^2\right\}\\
\log L &= \log\prod_{n=1}^{N} p(t_n|\mathbf{w},\mathbf{x}_n,\sigma^2)\\
&= \sum_{n=1}^{N}\log p(t_n|\mathbf{w},\mathbf{x}_n,\sigma^2)\\
&= \sum_{n=1}^{N}\log\left(\frac{1}{\sigma\sqrt{2\pi}}\right)-\sum_{n=1}^{N}\frac{1}{2\sigma^2}(t_n-\mathbf{w}^\mathsf{T}\mathbf{x}_n)^2\\
&= -N\log(\sigma\sqrt{2\pi})-\frac{1}{\sigma^2}\sum_{n=1}^{N}(t_n-\mathbf{w}^\mathsf{T}\mathbf{x}_n)^2
\end{aligned}
$$

Looks familiar!

Some re-arranging...

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&= -N\log(\sigma\sqrt{2\pi})-\frac{1}{\sigma^2}\sum_{n=1}^{N}(t_n-\mathbf{w}^\mathsf{T}\mathbf{x}_n)^2
\end{aligned}
$$

Looks familiar! To continue (good exercise):

$$
\frac{\partial\log L}{\partial\mathbf{w}}=0,\quad \frac{\partial\log L}{\partial\sigma^2}=0
$$

A shortcut

The multi-variate Gaussian

$$
\mathbf{y}=\begin{bmatrix} y_1\\ y_2\end{bmatrix},\quad p(\mathbf{y}|\boldsymbol{\mu},\boldsymbol{\Sigma})=\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})
$$

$$
\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})=\frac{1}{(2\pi)^{D/2}|\Sigma|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\mathsf{T}\boldsymbol{\Sigma}^{-1}(\mathbf{y}-\boldsymbol{\mu})\right\}
$$

D is number of variables, $|\boldsymbol{\Sigma}|$ is the determinant.

A shortcut

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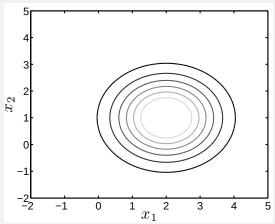

$$
\boldsymbol{\mu}=\begin{bmatrix}2\\1\end{bmatrix},\quad \boldsymbol{\Sigma}=\begin{bmatrix}1&0\\0&1\end{bmatrix}
$$

A shortcut

The multi-variate Gaussian

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \; p(\mathbf{y}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\Sigma|^{1/2}} \exp\left\{ -\frac{1}{2}(\mathbf{y} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu}) \right\}$$

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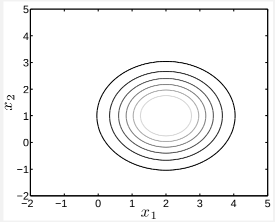

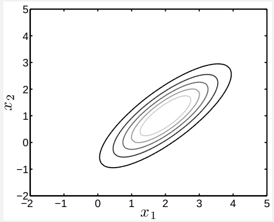

$$\boldsymbol{\mu} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \; \boldsymbol{\Sigma} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$

A shortcut

The multi-variate Gaussian

A special case:

$$\prod_{n=1}^{N} \mathcal{N}(\mu_n, \sigma^2) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_N \end{bmatrix}, \; \boldsymbol{\Sigma} = \begin{bmatrix} \sigma^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}$$

So, in our model:

$$\log L = \log \prod_{n=1}^{N} p(t_n|\mathbf{w}, \mathbf{x}_n, \sigma^2) = \log \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2\mathbf{I}) = \log p(\mathbf{t}|\mathbf{w}, \mathbf{X}, \sigma^2)$$

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Maximising the multi-variate log-likelihood

- Partial derivative w.r.t. $\mathbf{w}$, set to zero and solve:

$$\begin{aligned} \log L &= \log \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2\mathbf{I}) \\ \frac{\partial \log L}{\partial \mathbf{w}} &= -\frac{1}{2\sigma^2}(2\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{w} - 2\mathbf{X}^{\mathsf{T}}\mathbf{t}) = 0 \\ \mathbf{w} &= (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{t} \end{aligned}$$

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- This is the same expression we've seen before!

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- This is the same expression we've seen before!
- Same for σ^2:

$$\begin{aligned} \frac{\partial \log L}{\partial \sigma^2} &= -\frac{N}{2\sigma^2} + \frac{1}{(\sigma^2)^2}(\mathbf{t} - \mathbf{Xw})^\mathsf{T}(\mathbf{t} - \mathbf{Xw}) = 0 \\ \sigma^2 &= \frac{1}{N}(\mathbf{t} - \mathbf{Xw})^\mathsf{T}(\mathbf{t} - \mathbf{Xw}) \end{aligned}$$

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Optimum parameters

- Compute optimum $\widehat{\mathbf{w}}$ from:

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

- Use this to compute optimum $\widehat{\sigma^2}$ from:

$$\widehat{\sigma^2} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\widehat{\mathbf{w}})^\mathsf{T}(\mathbf{t} - \mathbf{X}\widehat{\mathbf{w}})$$

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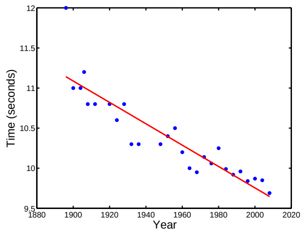
- e.g. Olympic 100 m data (again!)



$$\widehat{\mathbf{w}} = \begin{bmatrix} 36.416 \\ -0.0133 \end{bmatrix}, \quad \widehat{\sigma^2} = 0.0503$$

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Optimum parameters

- We have point estimates of our parameters.
- How confident should we be in them?
  - If we changed them a little bit, would the model still be good?

Confidence in parameter estimates

- Imagine there are **true** parameters, $\mathbf{w}$ and σ^2.

Confidence in parameter estimates

- Imagine there are **true** parameters, $\mathbf{w}$ and σ^2.
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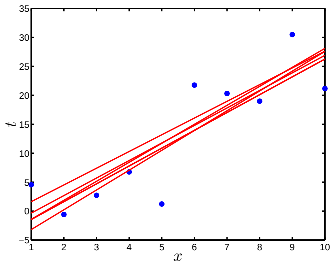

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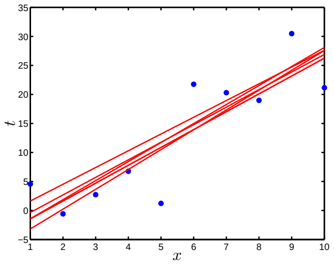

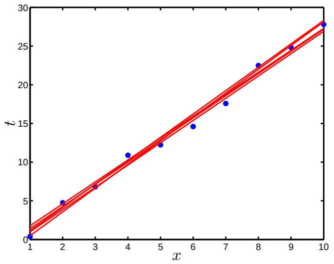

Summary

- Modelled the error as a random variable.
- Used a Gaussian random variable.
- Maximized the likelihood

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