Uncertainty in Deep Learning

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Bayesian Probabilistic Modelling (an Introduction)

Simple idea: *"If you're doing something which doesn't follow from the laws of probability, then you're doing it wrong"*

Structure

- From beliefs to ML
- On ML and 'assumptions'
- Generative story and probabilistic model
- Intuition: what does the likelihood really mean? (likelihood as a function of parameters)
- Intuition: The Posterior

From beliefs to ML

- I measured the temp this morning with my phone
- What do you think the temp could have been? (I don't want a single number!)

From beliefs to ML

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- I measured the temp this morning with my phone, **phone said 8c**
- My phone's temp sensor is noisy though.. (spec says it has 5c standard deviation)
- What do you think the actual temp was now?

From beliefs to ML

- We can write this down in maths
  - "I measured temp $x = 8$; sensor is noisy $\sigma = 5$; True temp μ?" We call this the likelihood [how I believe data/obs was generated given params]

$$X \mid \mu, \sigma = 5 \sim \mathcal{N}(\mu, \sigma^2).$$

- Since rational beliefs must follow the laws of prob theory, given our observation $x = 8$ we can encode our belief about what the true temp μ might have been using *Bayes law* [whiteboard]

$$\overbrace{p(\mu|\mathcal{D} = \{8\}, \sigma = 5)}^{\text{Posterior}} = \frac{\overbrace{p(\mathcal{D} = \{8\}|\mu, \sigma = 5)}^{\text{Likelihood}} \overbrace{p(\mu|\sigma = 5)}^{\text{Prior}}}{\underbrace{p(\mathcal{D} = \{8\}|\sigma = 5)}_{\text{Model evidence}}}$$

- The prior above is what I thought the temp might have been before making my obs, eg $\mu \sim \mathcal{N}(5, 10)$

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From beliefs to ML

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- I made a **second** measurement with my phone, and this time it said 13c
- Remember: phone's temp sensor is noisy.. (5c standard deviation)
- What do you think the actual temp μ was now?

From beliefs to ML

- Our posterior belief from before is our new *prior belief*

$$\overbrace{p(\mu|\mathcal{D}=\{8\},\sigma=5)}^{\text{Prior}}$$

- Which, given the new obs $x = 13$, we must update using the laws of probability:

$$\overbrace{p(\mu|\mathcal{D}=\{13,8\},\sigma=5)}^{\text{Posterior}}$$

$$= \frac{\overbrace{p(\mathcal{D}=\{13\}|\mu,\mathcal{D}=\{8\},\sigma=5)}^{\text{Likelihood}}\overbrace{p(\mu|\mathcal{D}=\{8\},\sigma=5)}^{\text{Prior}}}{\underbrace{p(\mathcal{D}=\{13\}|\mathcal{D}=\{8\},\sigma=5)}_{\text{Model evidence}}}$$

- And so on... (we'll see soon how to eval these things)

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Probabilistic Modelling and Assumptions

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Above is an example of encoding our assumptions into a *model*.

- can't do ML without **assumptions**
  - there always exists some **underlying process** that generated obs
  - **all models** make assumptions about this process, either explicitly, or implicitly
  - in Bayesian probabilistic modelling we make our assumptions about underlying process **explicit**
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- eg – astrophysics: gravitational lensing
  - there exists a physics process magnifying far away galaxies
  - Nature chose lensing coeff $\rightarrow$ gravitational lensing mechanism $\rightarrow$ transform galaxy
  - We **observe** transformed galaxies, want to **infer** lensing ceoff

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- eg – cats vs dogs classification
  - there exist some underlying rules we don't know
  - eg "if has pointy ears then cat"
  - We **observe** pairs (image, "cat"/"no cat"), and want to **infer** underlying mapping from images to labels

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- eg – Gaussian density estimation
  - I tell you the process I used to generate data and give 5 data points

$$x_n \sim \mathcal{N}(x_n; \mu, \sigma^2), \qquad \sigma = 1$$

  - you **observe** the points $\{x_1, ..., x_5\}$, and want to **infer** my μ
  - Reminder: Gaussian density with mean μ and variance σ^2

$$p(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

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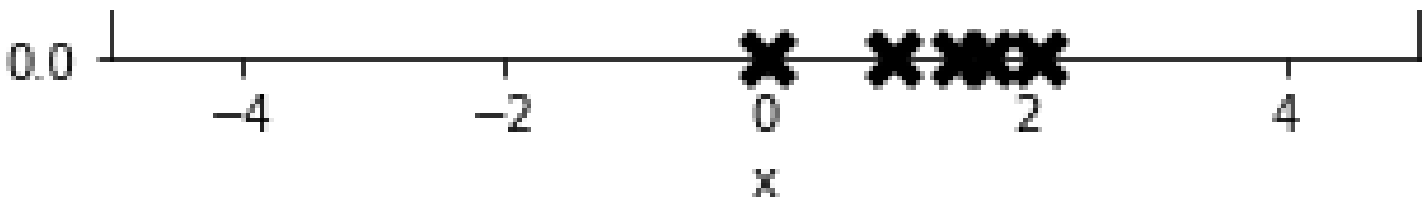

X Which μ generated my data?

V What's the probability that $\mu = 10$ generated my data? (want to infer distribution over μ!)

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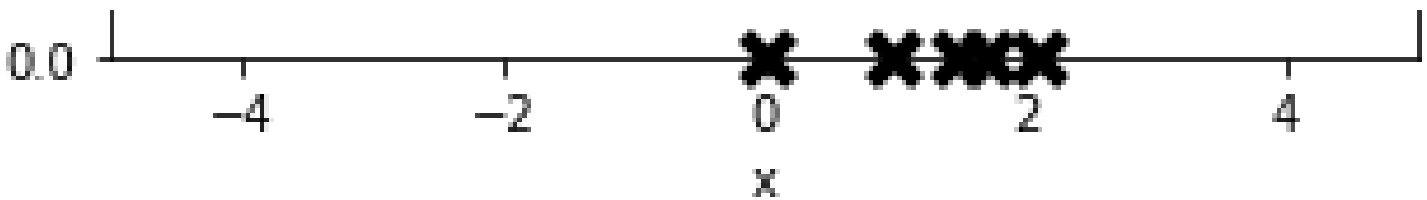

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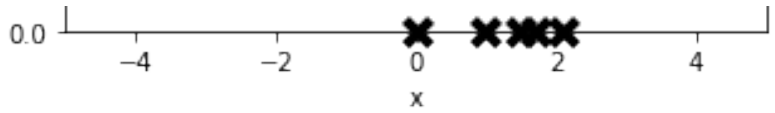
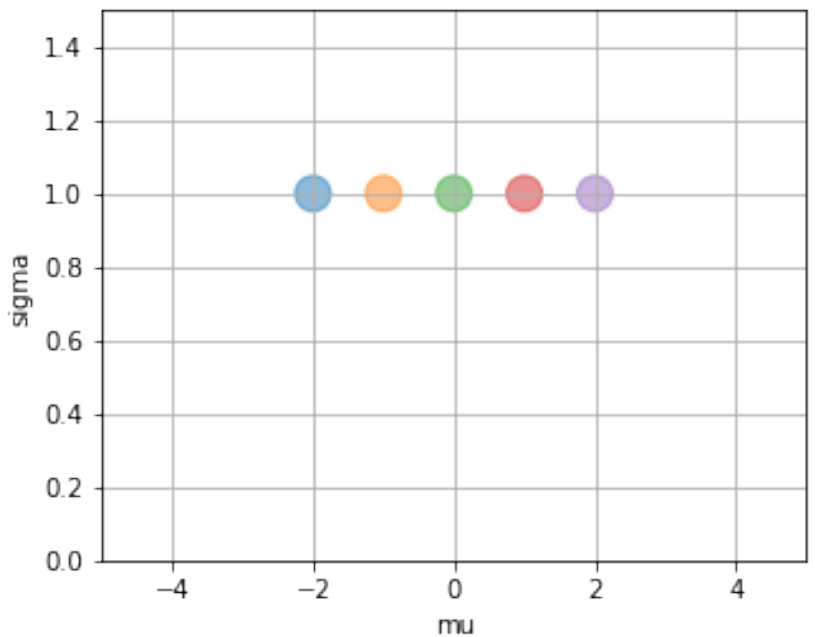


- These are the hypotheses we'll play with: (in parameter space)



- I chose a Gaussian (one of those) from which I generated my data
- Which Gaussian do you think I chose?

Probabilistic Modelling and Assumptions

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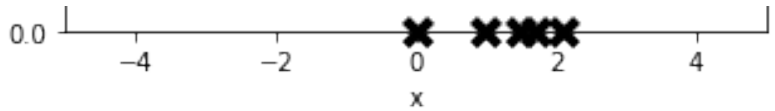
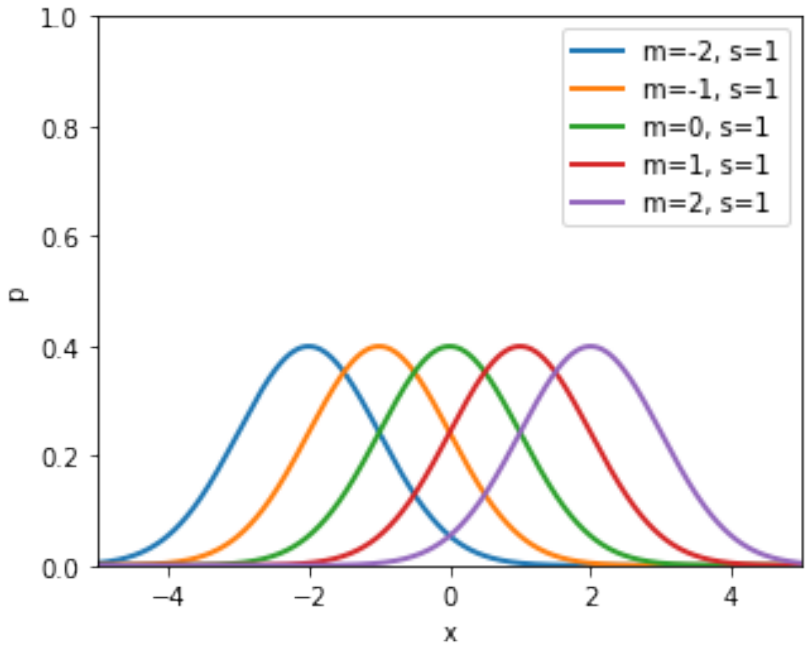


- And this is what the hypotheses look like in data space:



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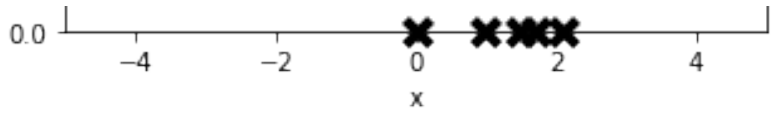

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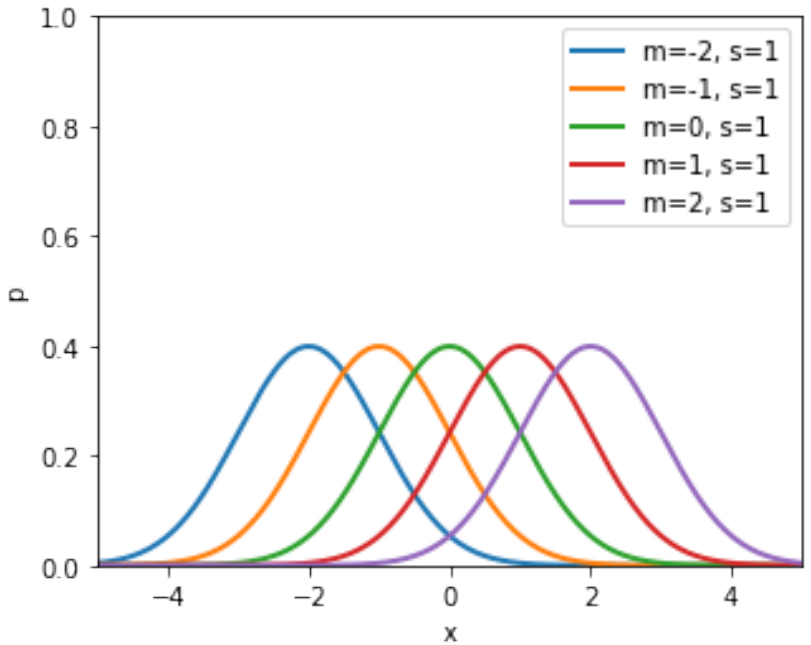

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Generative story / probabilistic model

In Bayesian probabilistic modelling

- want to represent our beliefs / assumptions about how data was generated explicitly
- eg via *generative story* ['*My assumptions are...*']:
  - Someone (me / Nature / etc) selected parameters μ, σ
  - Generated N data points $x_n \sim \mathcal{N}(\mu, \sigma^2)$
  - Gave us $\mathcal{D} = \{x_1, ..., x_N\}$ (and also $\sigma = 1$)

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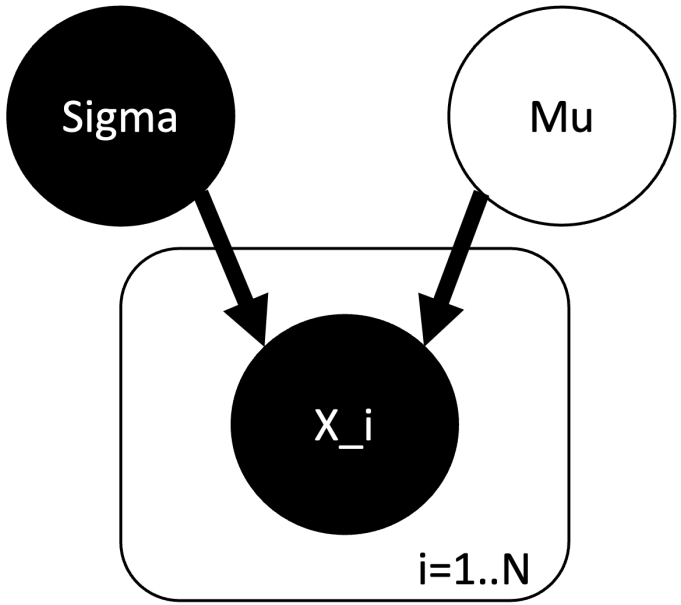
Generative story

- Can represent generative story pictorially as a *plate diagram* (also known as a Bayesian network / graphical model)



  - Circle = random variable
  - Plate = repetition
  - Black = observed; white = unobserved
  - Arrows = conditional dependence

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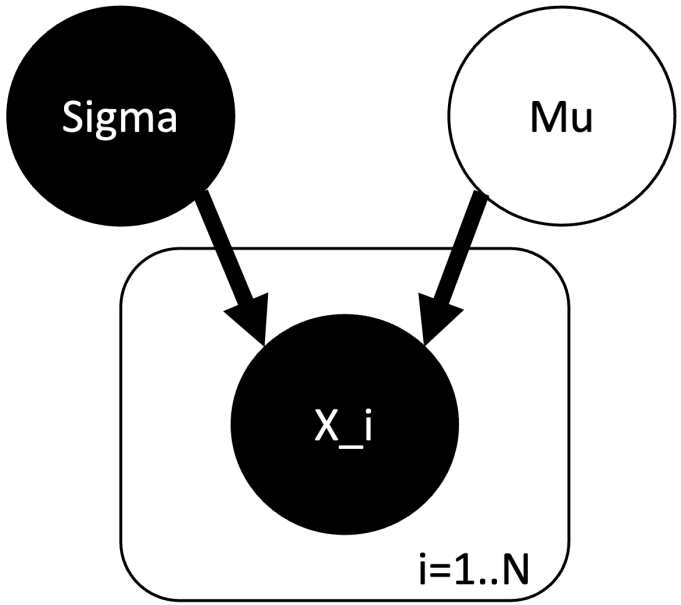

- This represents how we believe our data was generated – what depends on what
- we're given σ, there exists *some* μ, and our observed x_i's are dependent on both
  - eg, x_1 not dependent on x_2 when we condition on μ and σ
  - ? does x_1 depend on x_2 when we **don't** condition on μ and σ?

Joint distribution

Mathematically, this corresponds to this joint distribution:

$$p(\mathcal{D} = \{x_1, .., x_N\}, \mu, \sigma) = p(\mathcal{D} = \{x_1, .., x_N\}|\mu, \sigma) \cdot p(\mu) \cdot p(\sigma)$$

with (product rule)

$$p(\mathcal{D} = \{x_1, .., x_N\}|\mu, \sigma) = \prod_{i=1}^{N} p(x_i|\mu, \sigma)$$

? what does the joint look like with no conditional independence (factorisation) assumption?

We haven't specified what these distributions are yet... (e.g., what's $p(\mu)$?)

Generative story $\rightarrow$ probabilistic model

We can build a Bayesian probabilistic model following this generative story:

- prior [what I believe params might look like]

$$\mu \sim \mathcal{N}(0, 10), \qquad \sigma = 1$$

- likelihood [how I believe data was generated given params]

$$x_n \mid \mu, \sigma \sim \mathcal{N}(\mu, \sigma^2), \qquad n = 1..N$$

And plug these into the above joint distribution:

$$p(x_n|\mu, \sigma) = \mathcal{N}(x_n; \mu, \sigma^2)$$

$$p(\mu) = \mathcal{N}(\mu; 0, 10)$$

and

$$p(\sigma) = \delta(\sigma = 1)$$

(σ equals 1 with prob 1)

Generative story / probabilistic model (Exercise)

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Exercise: Draw a plate diagram, write the joint probability, and build a prob model for this generative story

My assumptions are...

- Someone (me / Nature / etc) selected parameters $\mu_n \in \mathbb{R}^{10}, \sigma_n \in \mathbb{R}^+$ for $n = 1..N$, and decoder function $f : \mathbb{R}^{10} \to X$
- Generated N latent points $z_n \sim \mathcal{N}(\mu_n, \sigma_n^2)$
- Decoded these z's and generated N data points $x_n \sim \mathcal{N}(f(z_n), 1)$
- Gave us $f, \mathcal{D} = \{x_1, ..., x_N\}$

Can you find my Gaussian?

Going back to our simple case, how can we update prior belief on μ conditioned on data you give me? (infer posterior distribution over $\mu \mid \{x_1, ..., x_N\}$)

Everything follows the **laws of prob**..

- Sum rule

$$p(X = x) = \sum_y p(X = x, Y = y) = \int p(X = x, Y) \mathrm{d}Y$$

- Product rule

$$p(X = x, Y = y) = p(X = x | Y = y) p(Y = y)$$

- Bayes rule

$$p(X = x | Y = y, \mathcal{H}) = \frac{p(Y = y | X = x, \mathcal{H}) p(X = x | \mathcal{H})}{p(Y = y | \mathcal{H})}$$

Note: $\mathcal{H}$ is often omitted in conditional for brevity

Updating our beliefs (Inference)

Bayes rule:

$$p(X = x|Y = y, \mathcal{H}) = \frac{p(Y = y|X = x, \mathcal{H})p(X = x|\mathcal{H})}{p(Y = y|\mathcal{H})},$$

and in probabilistic modelling:

$$\overbrace{p(\mu|\mathcal{D}, \sigma, \mathcal{H})}^{\text{Posterior}} = \frac{\overbrace{p(\mathcal{D}|\mu, \sigma, \mathcal{H})}^{\text{Likelihood}}\overbrace{p(\mu|\sigma, \mathcal{H})}^{\text{Prior}}}{\underbrace{p(\mathcal{D}|\sigma, \mathcal{H})}_{\text{Model evidence}}}$$

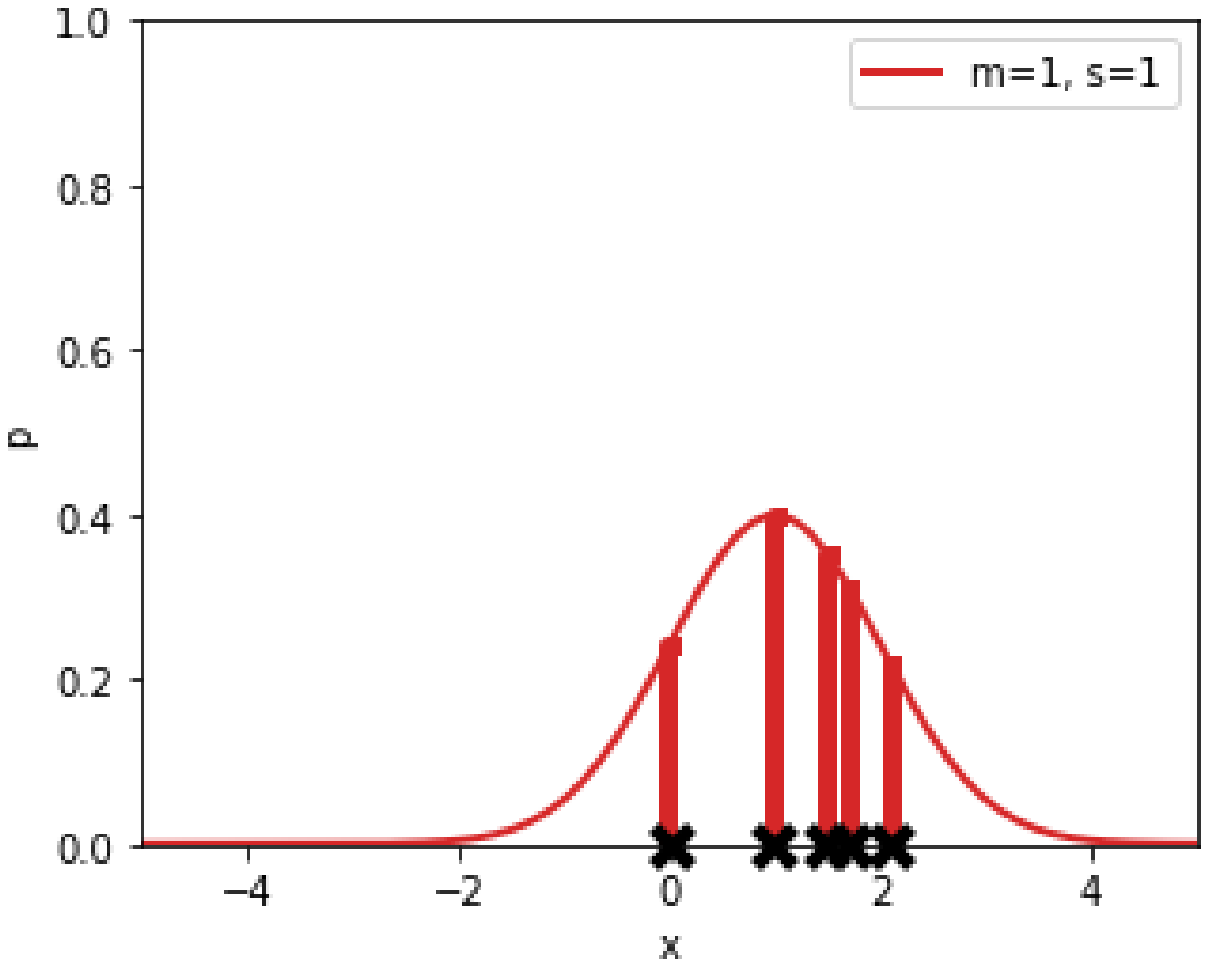
with model evidence $p(\mathcal{D}|\sigma, \mathcal{H}) = \int p(\mathcal{D}|\mu, \sigma, \mathcal{H})p(\mu|\sigma, \mathcal{H})\mathrm{d}\mu$ (sum rule).

Let's look into each one of these quantities in more detail.

The Likelihood in more detail: Intuition

Likelihood $p(\mathcal{D}|\mu, \sigma, \mathcal{H})$

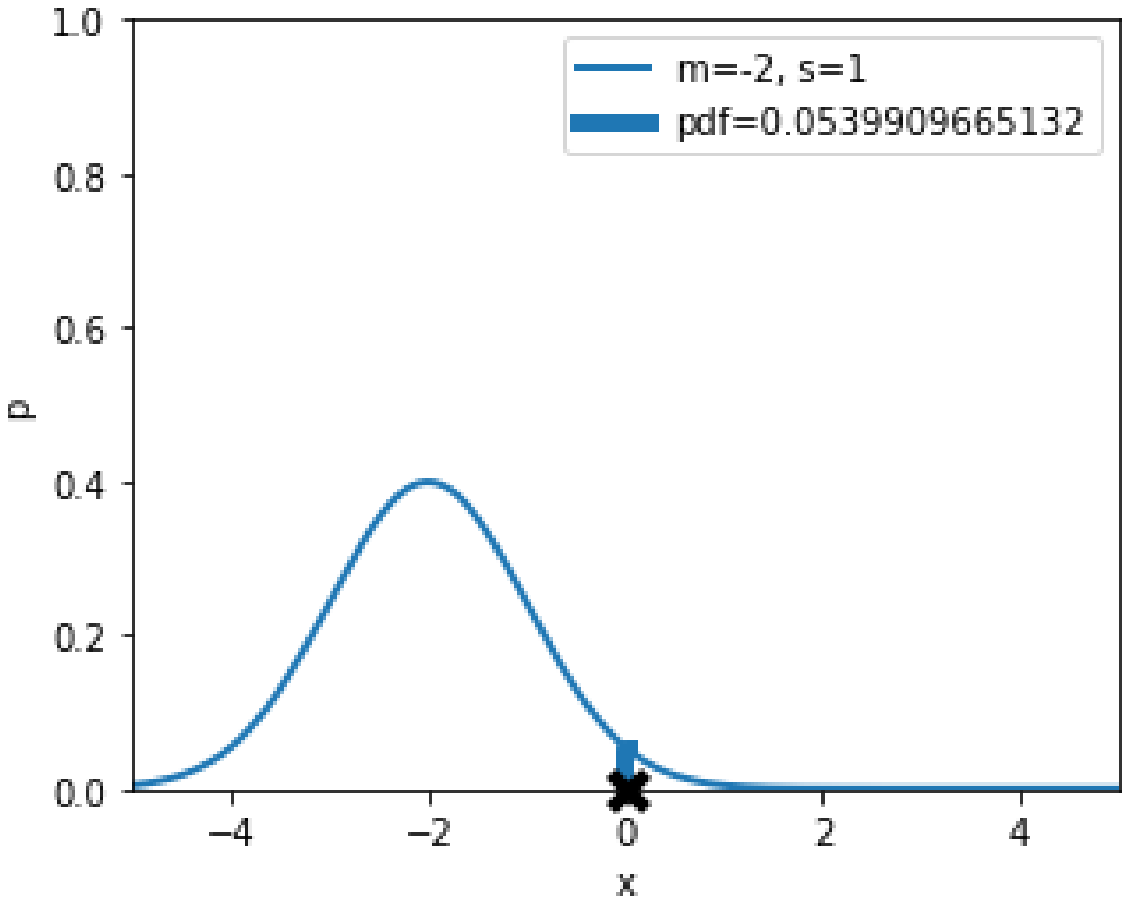
- we explicitly assumed data comes iid from a Gaussian
- compute $p(\mathcal{D}|\mu, \sigma)$ = multiply all $p(x_n|\mu, \sigma)$ (product rule)



Likelihood as a function of parameters

Let's look in detail – reducing dataset from 5 points to 1:

- What does the likelihood look like? let's 'scan' the parameter space



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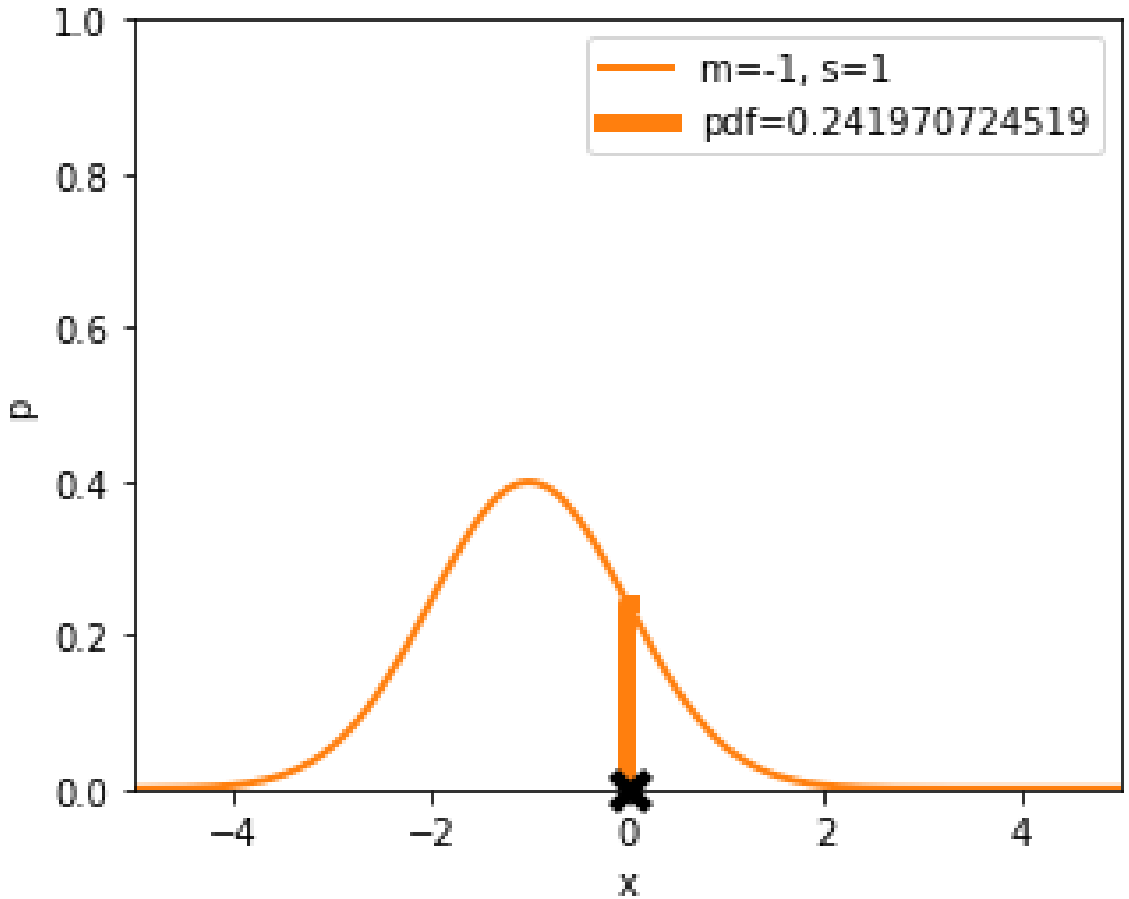

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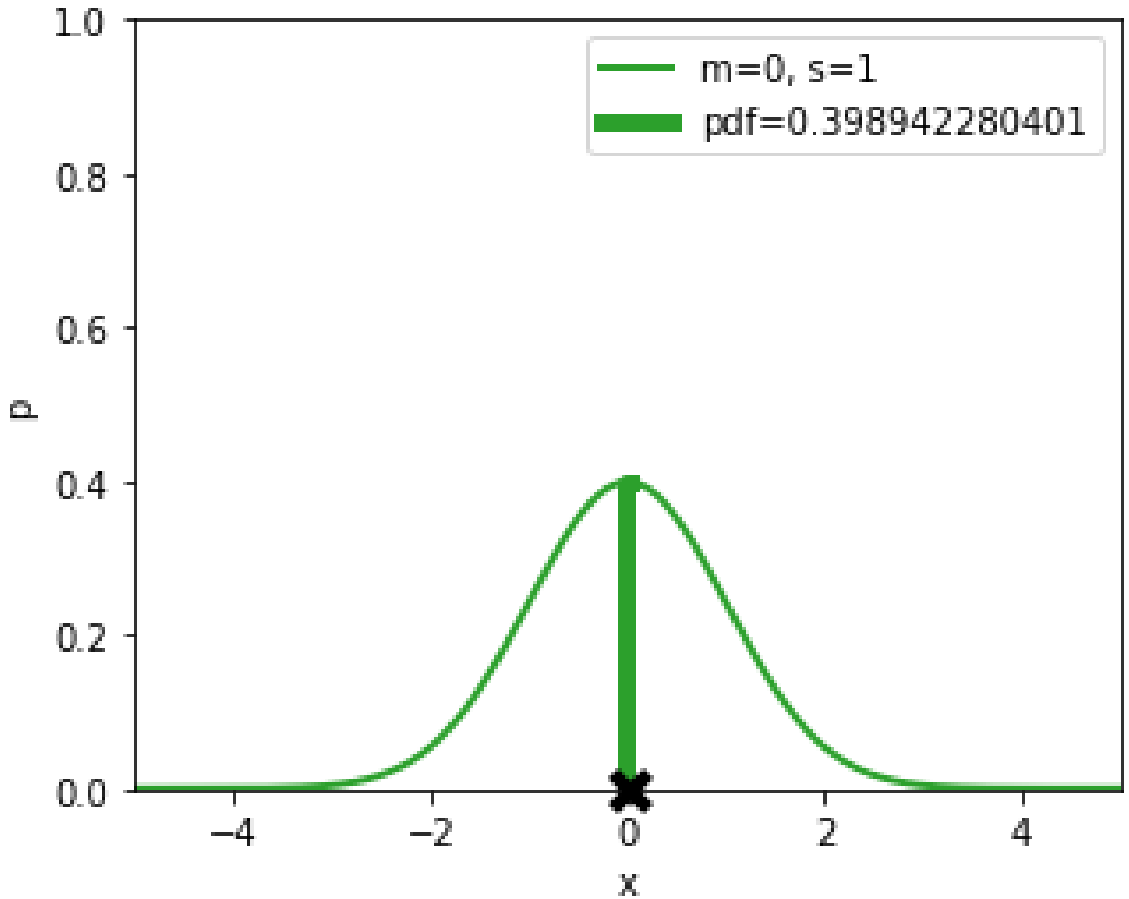

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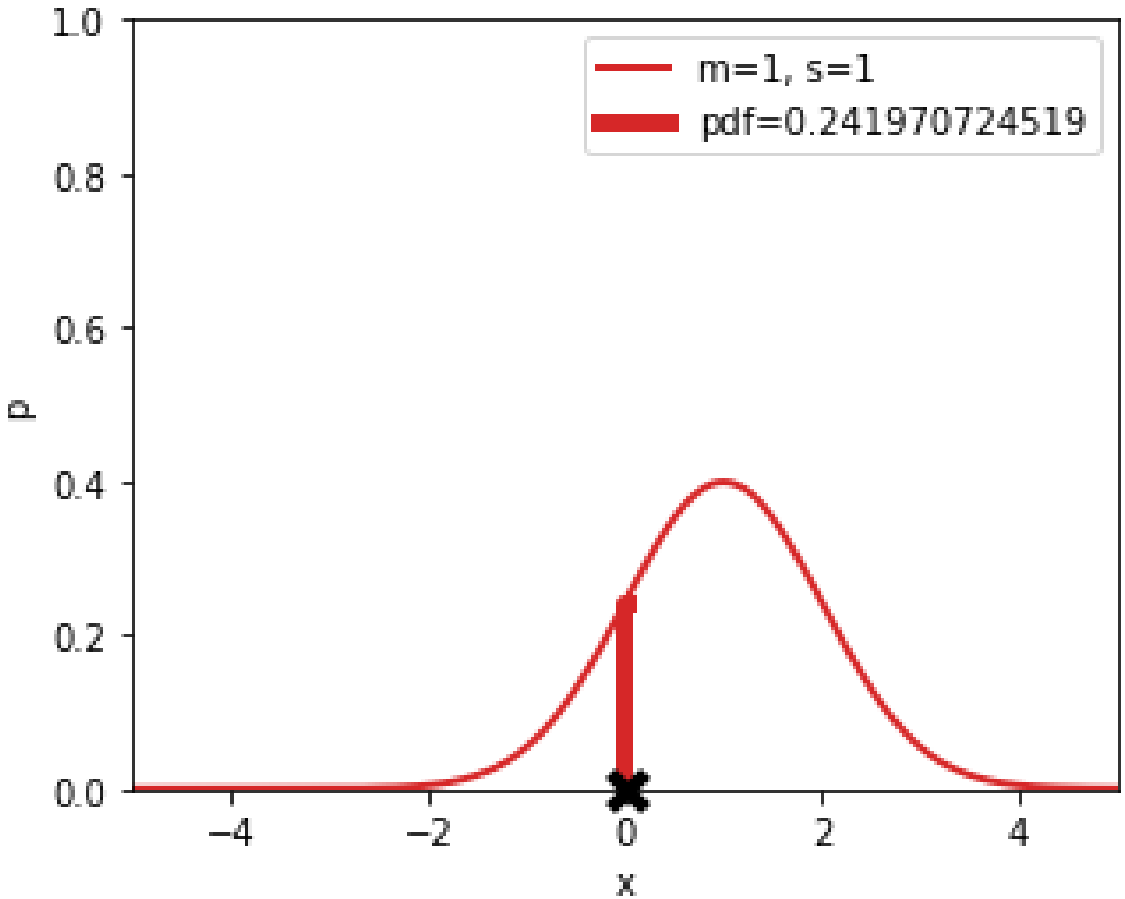

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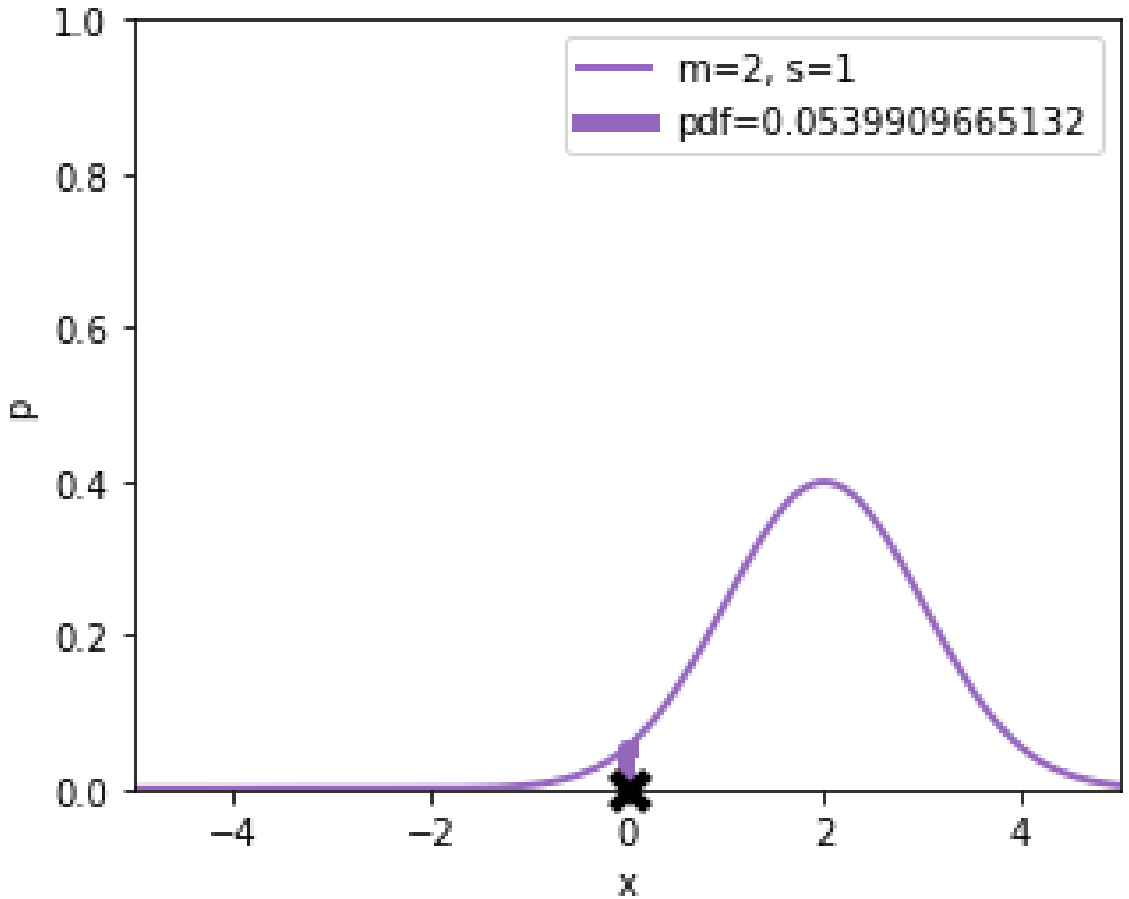

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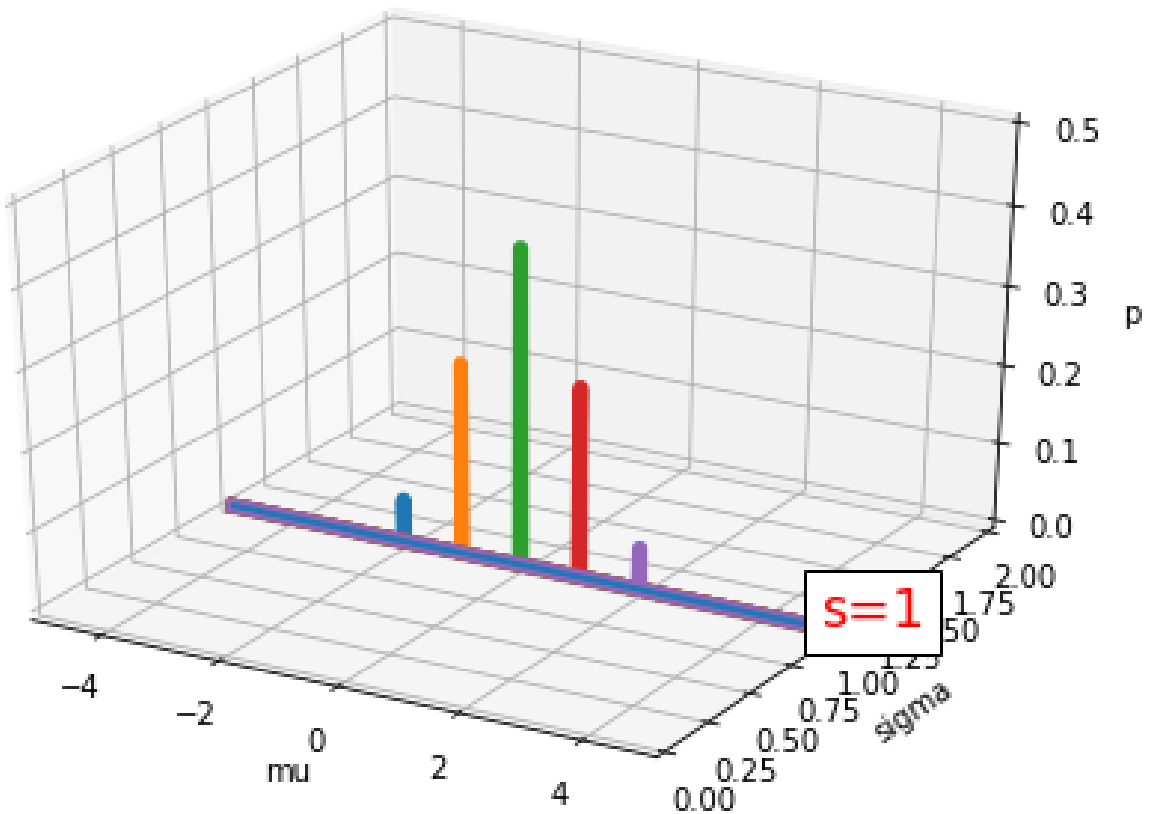
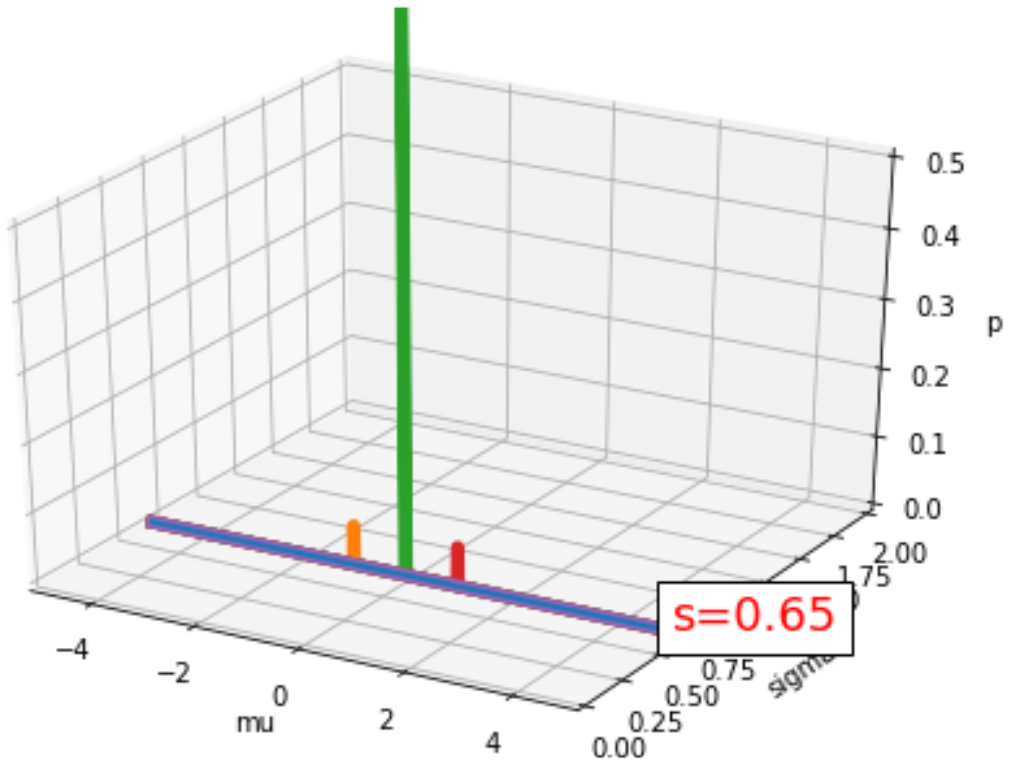
  This is what the likelihood look like as a *function* of the params



Likelihood as a function of parameters

Let's look in detail – reducing dataset from 5 points to 1:

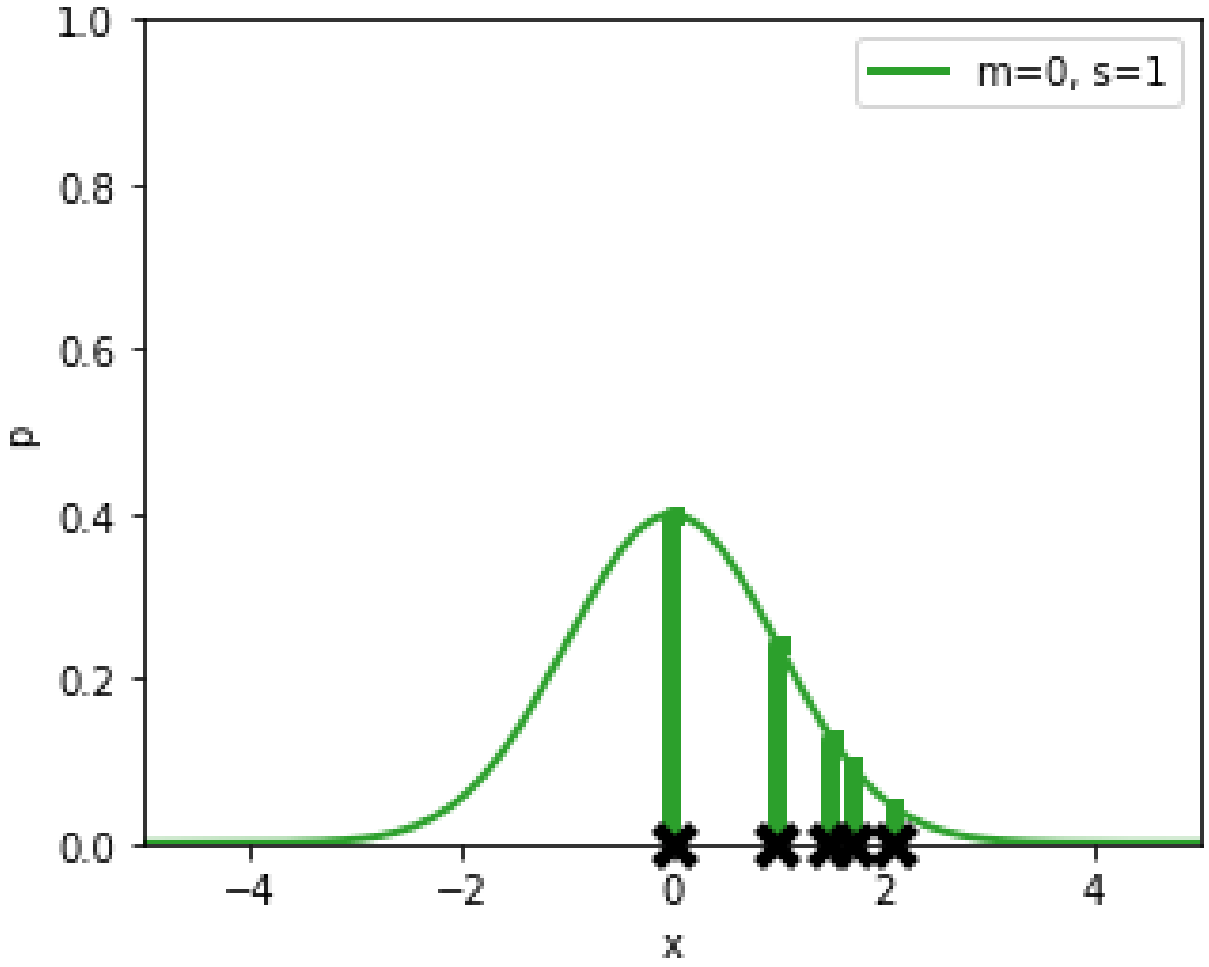
- What does the likelihood look like? let's 'scan' the parameter space and with smaller σ..



- MLE (max lik) will get "absolutely certain that $\sigma = 0$ & $\mu = 0$"
- Does this make sense? (I **told** you $x_n \sim \mathcal{N}$!)
- MLE failure

Likelihood as a function of parameters

And now scanning with all data, computing product of likelihoods:



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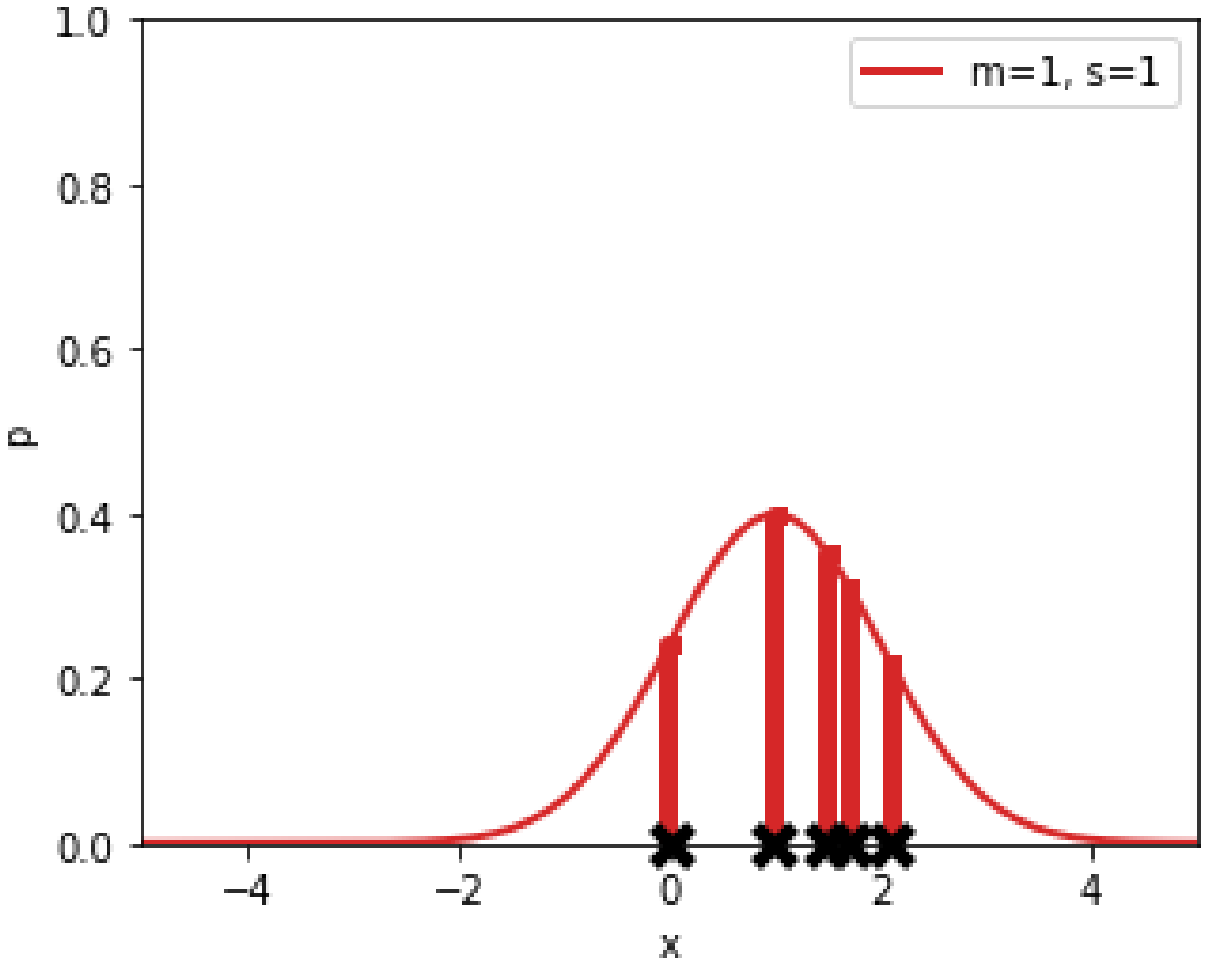

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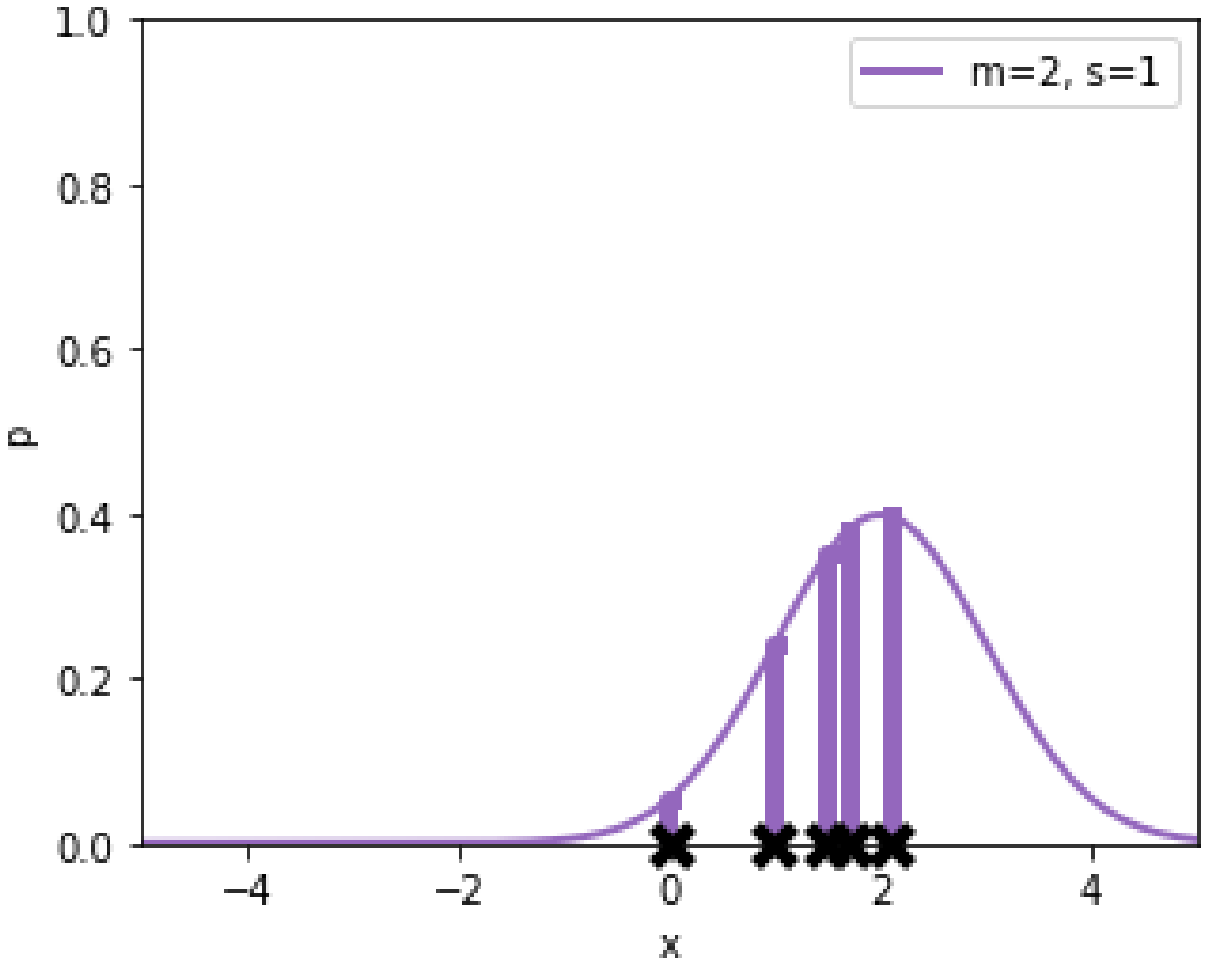
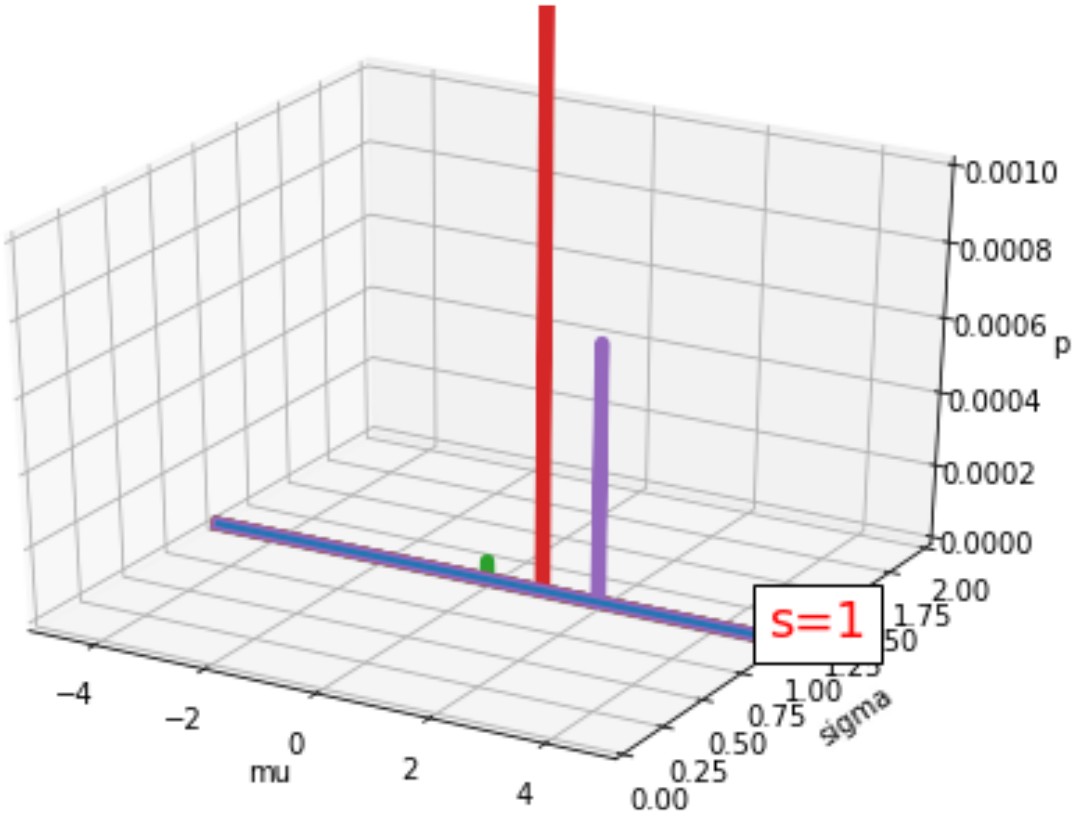


Likelihood as a function of parameters

And now scanning with all data, computing product of likelihoods:



Likelihood function tells us how well every value of μ, σ predicted what would happen.

The Posterior in more detail

$$\overbrace{p(\mu|\mathcal{D},\sigma,\mathcal{H})}^{\text{Posterior}} = \frac{\overbrace{p(\mathcal{D}|\mu,\sigma,\mathcal{H})}^{\text{Likelihood}}\overbrace{p(\mu|\sigma,\mathcal{H})}^{\text{Prior}}}{\underbrace{p(\mathcal{D}|\sigma,\mathcal{H})}_{\text{Model evidence}}}$$

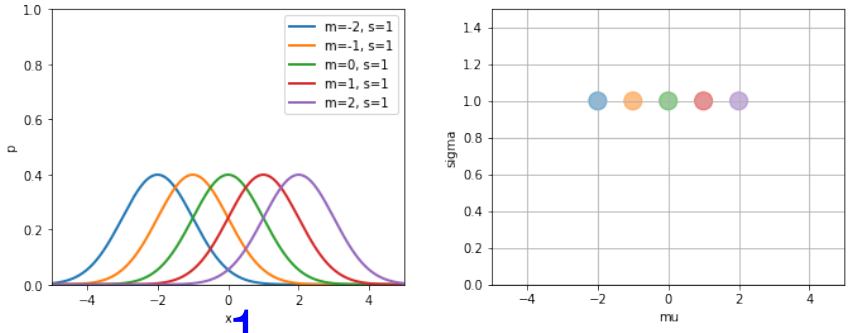
In contrast to the likelihood, posterior would say

'*with the data you gave me and prior assumptions, this is what I think μ could be, and I might become more confident if you give me more data*'

- normaliser = **marginal** likelihood = evidence = sum of likelihood * prior
  - $$p(\mathcal{D}|\sigma,\mathcal{H}) = \int p(\mathcal{D},\mu|\sigma,\mathcal{H})\mathrm{d}\mu \text{ (sum rule)}$$
    $$= \int p(\mathcal{D}|\mu,\sigma,\mathcal{H})p(\mu|\sigma,\mathcal{H})\mathrm{d}\mu \text{ (product rule)}$$
  - (but often difficult to calculate... more in the next lecture)

The Posterior in more detail

- Eg, inference w prior = 'we believe data is equally likely to have come from one of the 5 Gaussians w $\sigma = 1$'



$$p(\mu = \mu_i|\sigma, \mathcal{H}) = \frac{1}{5} \text{ and } p(\mu \neq \mu_i \text{ for all } i|\sigma, \mathcal{H}) = 0$$

then marginal likelihood is

$$p(\mathcal{D}|\sigma, \mathcal{H}) = \sum_i p(\mathcal{D}|\mu = \mu_i, \sigma, \mathcal{H}) p(\mu = \mu_i|\sigma, \mathcal{H})$$

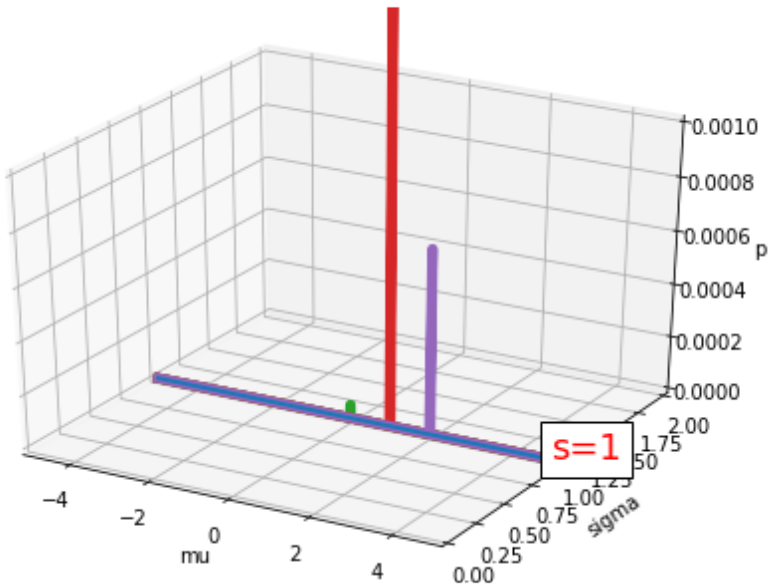
$$= \sum_i p(\mathcal{D}|\mu = \mu_i, \sigma, \mathcal{H}) \frac{1}{5}$$

and posterior is

$$p(\mu = \mu_i|\sigma, \mathcal{D}, \mathcal{H}) = \frac{1/5 p(\mathcal{D}|\mu = \mu_i, \sigma, \mathcal{H})}{\sum_i 1/5 p(\mathcal{D}|\mu = \mu_i, \sigma, \mathcal{H})}$$

The Posterior in more detail

Using likelihood from above, our **posterior distribution** over μ (prob of different values for μ given the observed data) is given by:



Some useful terminology we will use in the future:

- marginal likelihood of sigma=1 = $p(\mathcal{D}|\sigma = 1, \mathcal{H})$ = 'prob that data came from single Gaussian with param $\sigma = 1$'
- similarly, marginal likelihood of hypothesis = $p(\mathcal{D}|\mathcal{H})$ = 'prob that data came from single Gaussian (with some μ, σ)'

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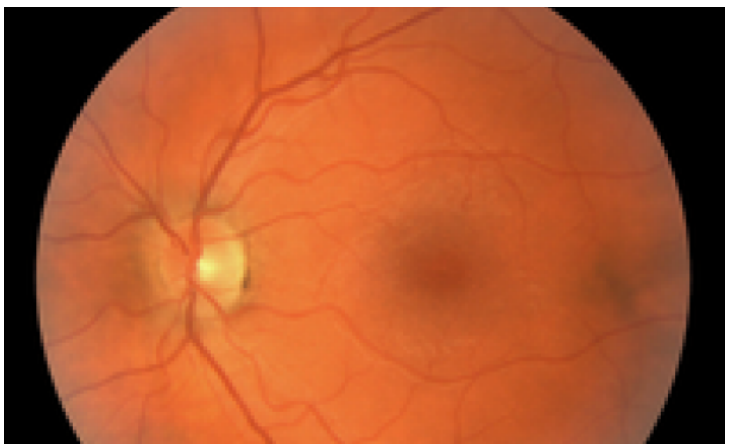
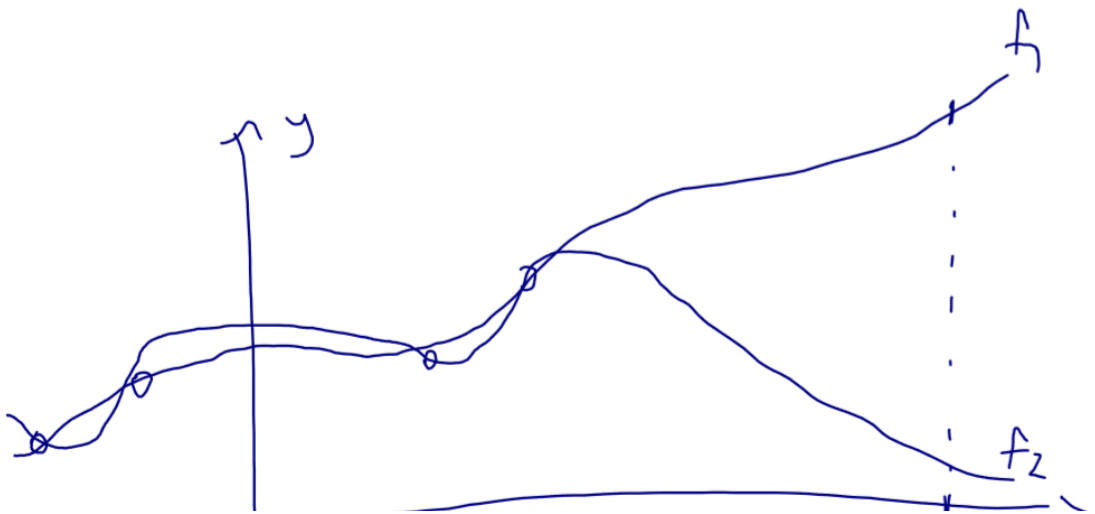
Bayesian Probabilistic Modelling of Functions

Structure

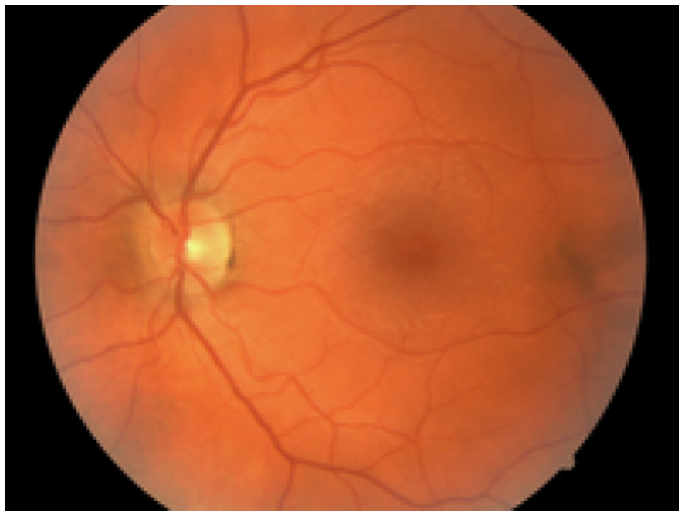
- Why uncertainty over functions
- Linear regression
- Linear basis function regression
- Parametrised basis functions
- Hierarchy of parametrised basis functions (aka neural networks)
- NNs through a probabilistic lens (generative story, prob model, inference, predictions)

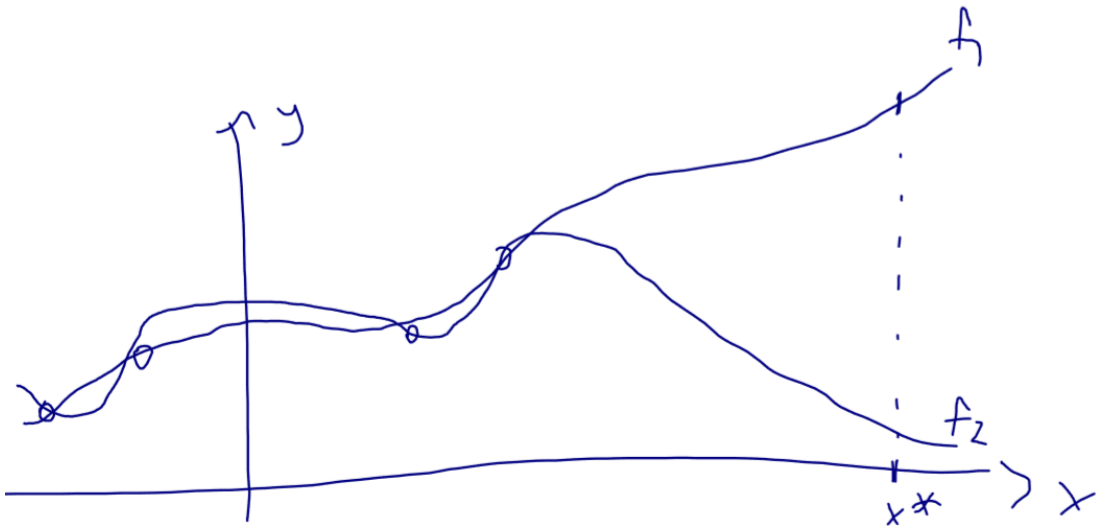




Why uncertainty over functions

- Going beyond beliefs over discrete set of bets ('heads happened') / scalars (μ)





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- Distribution over weights = dist over *functions*
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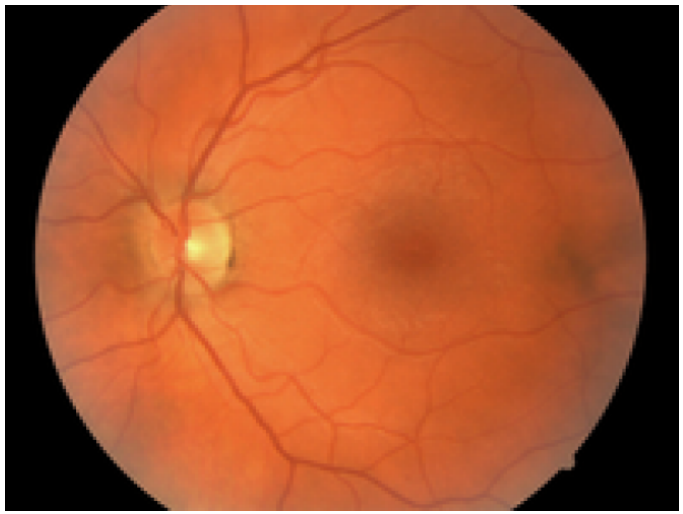

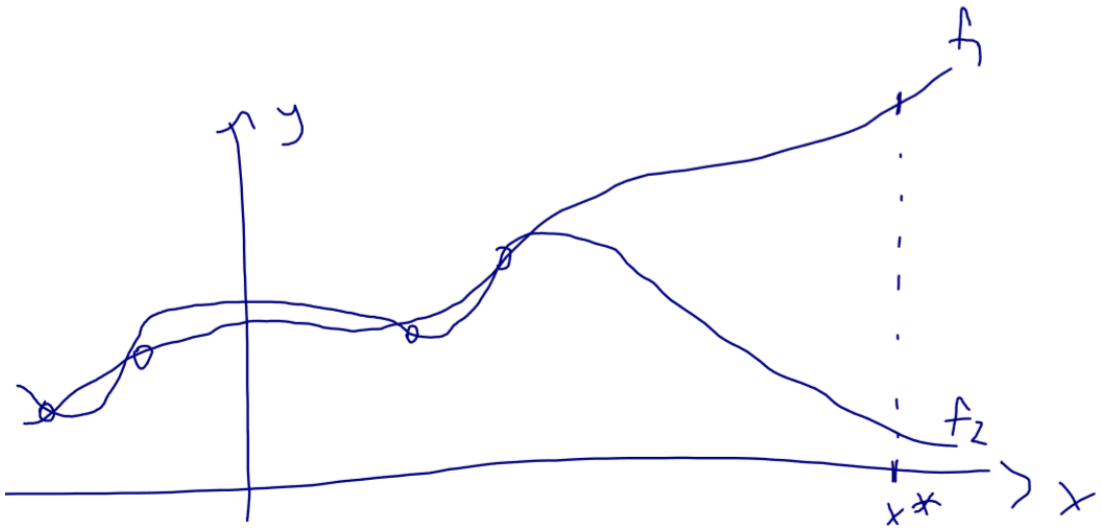

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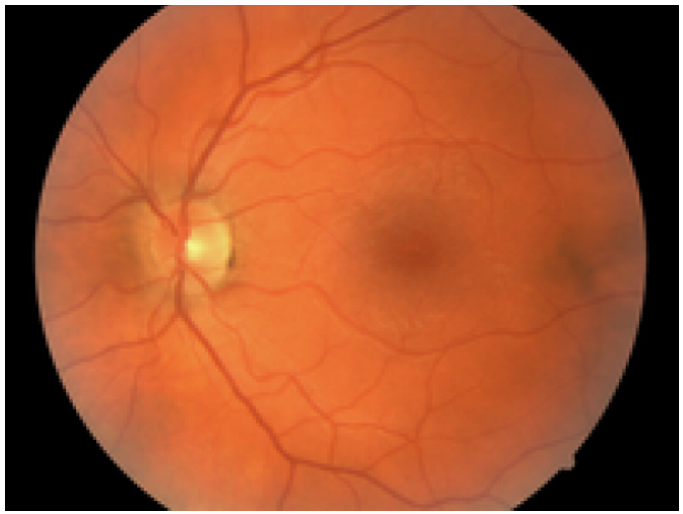

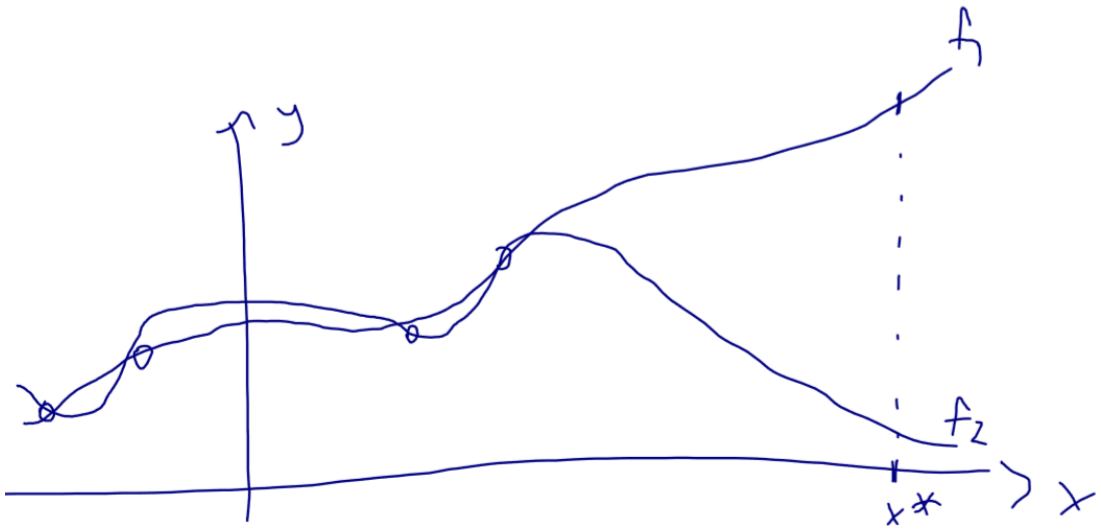

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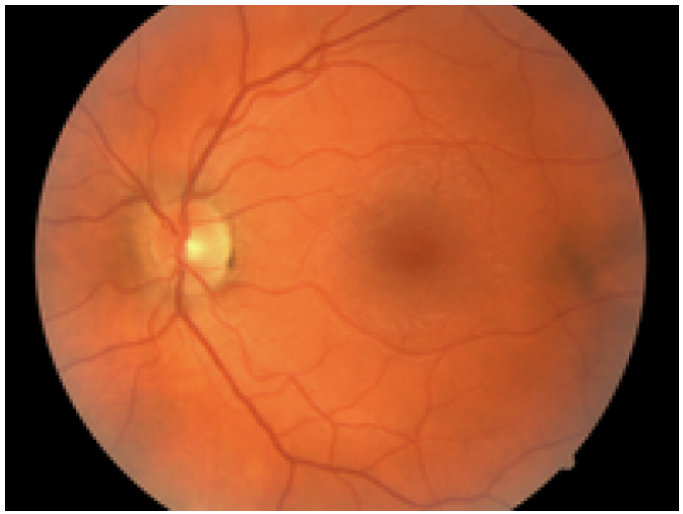

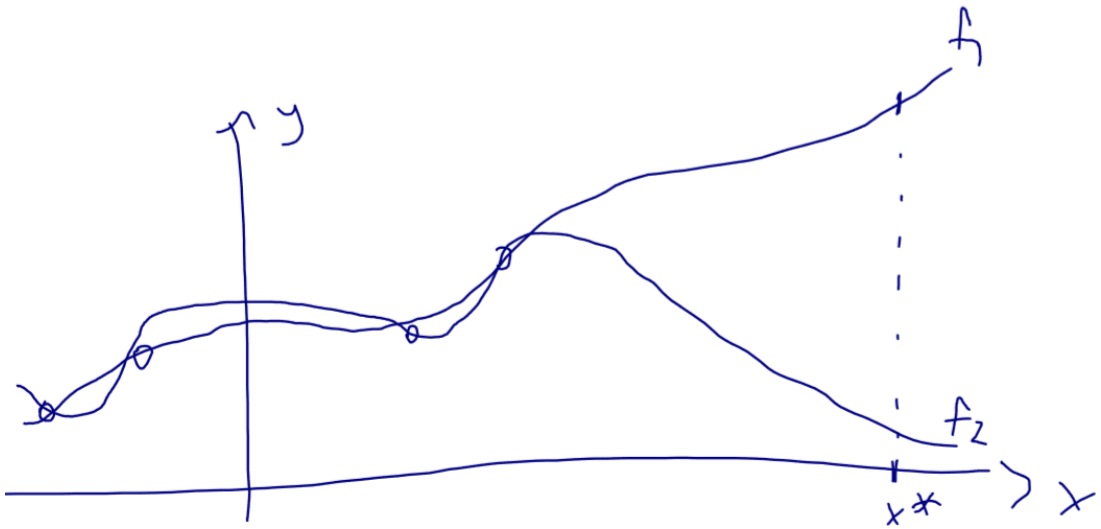

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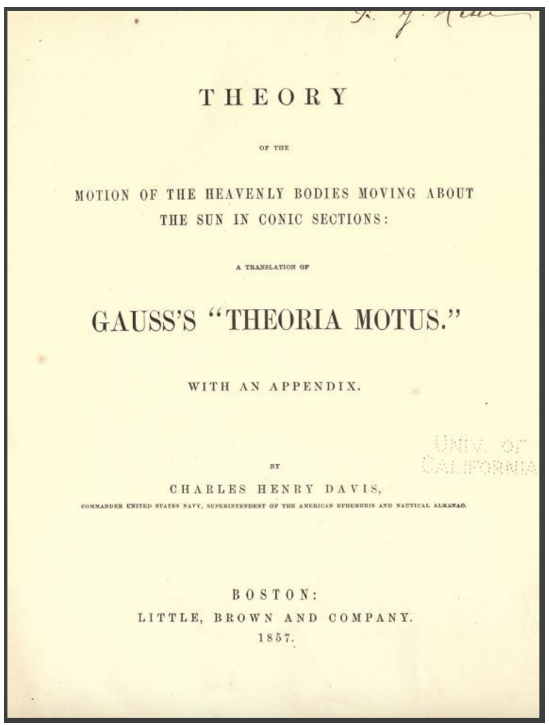

THEORY

OF THE

MOTION OF THE HEAVENLY BODIES MOVING ABOUT THE SUN IN CONIC SECTIONS:

A TRANSLATION OF

GAUSS'S "THEORIA MOTUS."

WITH AN APPENDIX.

BY

CHARLES HENRY DAVIS,

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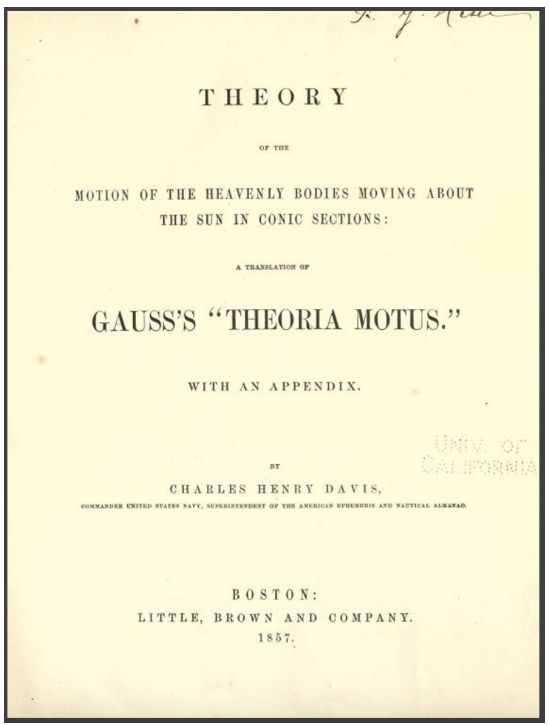

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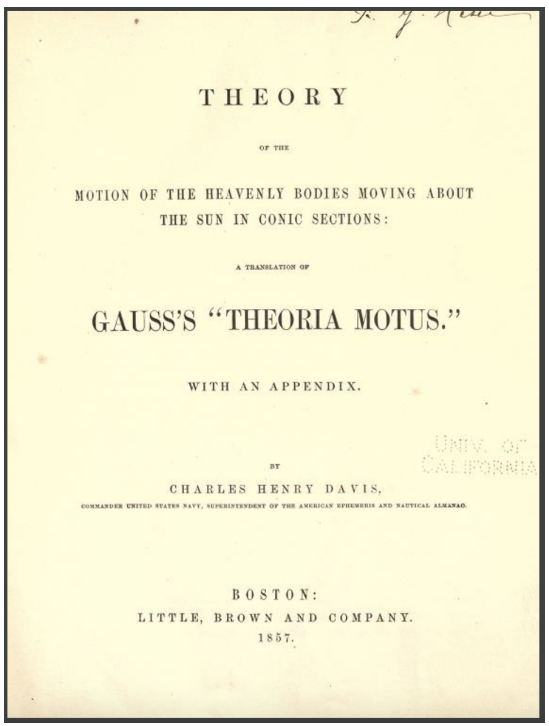

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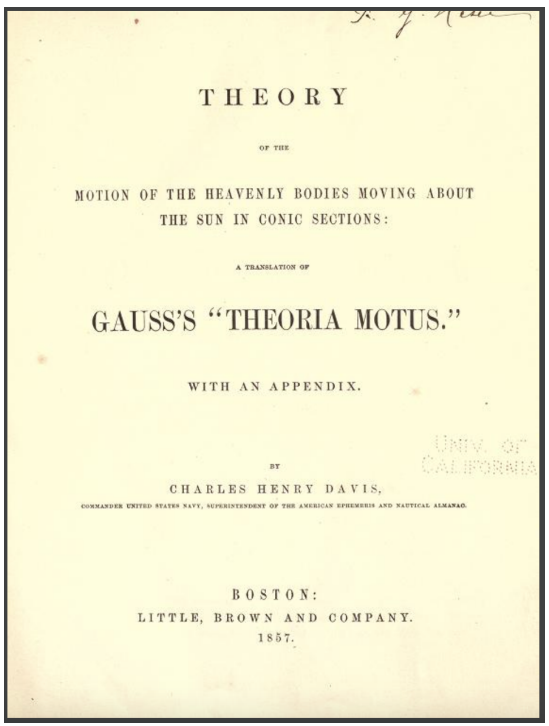

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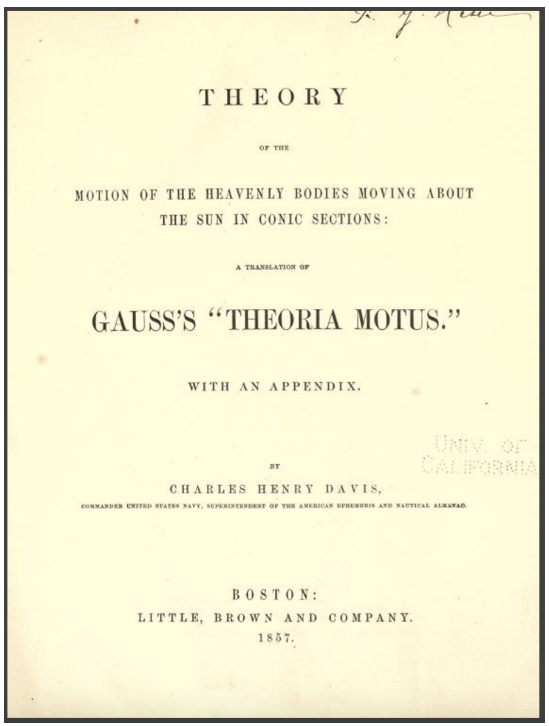

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and S.M. Stigler, University of Wisconsin

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  - sinusoidals with various frequencies: $\sin(kx)$
  - wavelets parametrised by k: $\cos(k\pi x)e^{-x^2/2}$
- collect into a **feature vector** $\varphi(\mathbf{x}) = [\varphi_1(\mathbf{x}), ..., \varphi_K(\mathbf{x})]$, e.g.

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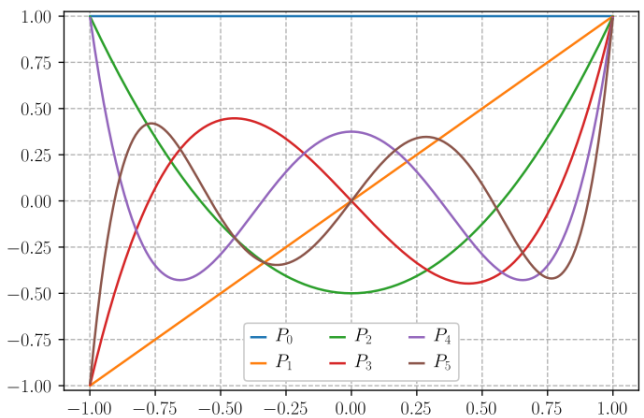

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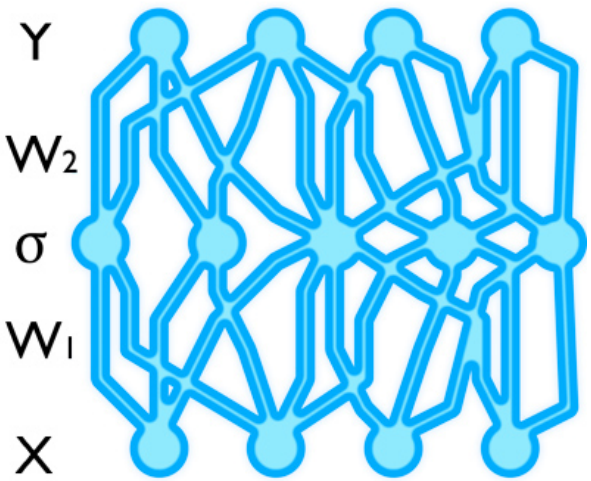
Parametrised basis functions [Bishop, 2006]

- eg basis functions $\varphi_k^{w_k,b_k}$ where scalar-valued function φ_k is applied to inner-product $w_k^T \mathbf{x} + b_k$
  - φ_k often def'd to be identical for all k (only params change)
  - eg $\varphi_k(\cdot) = \tanh(\cdot)$, giving $\varphi_k^{w_k,b_k}(\mathbf{x}) = \tanh(w_k^T \mathbf{x} + b_k)$
- feature vector = basis functions' outputs = input to linear trans.
- in vector form:
  - W_1 a matrix of dimensions Q by K
  - b_1 a vector with K elements
  - $\varphi^{W_1,b_1}(\mathbf{x}) = \varphi(W_1 \mathbf{x} + b_1)$
  - W_2 a matrix of dimensions K by D
  - b_2 a vector with D elements
  - model output: $f^{W_1,b_1,W_2,b_2}(\mathbf{x}) = \varphi^{W_1,b_1}(\mathbf{x}) W_2 + b_2$
- want to find W_1, b_1, W_2, b_2 that minimise $1/N \sum_i ||\mathbf{y}_i - f^{W_1,b_1,W_2,b_2}(\mathbf{x}_i)||^2$



Parametrised basis functions [Bishop, 2006]

- eg basis functions $\varphi_k^{w_k,b_k}$ where scalar-valued function φ_k is applied to inner-product $w_k^T \mathbf{x} + b_k$
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- feature vector = basis functions' outputs = input to linear trans.
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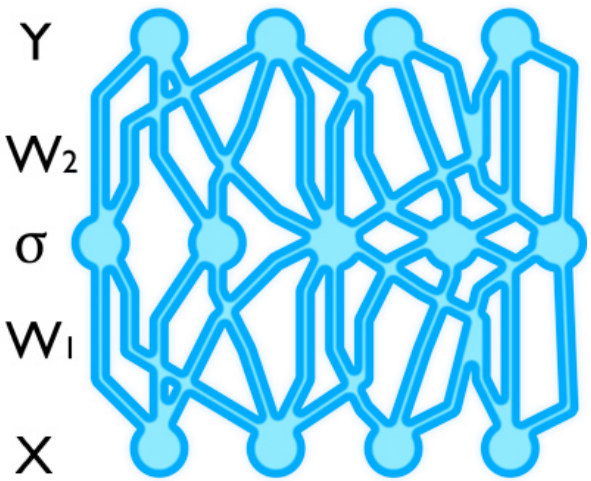

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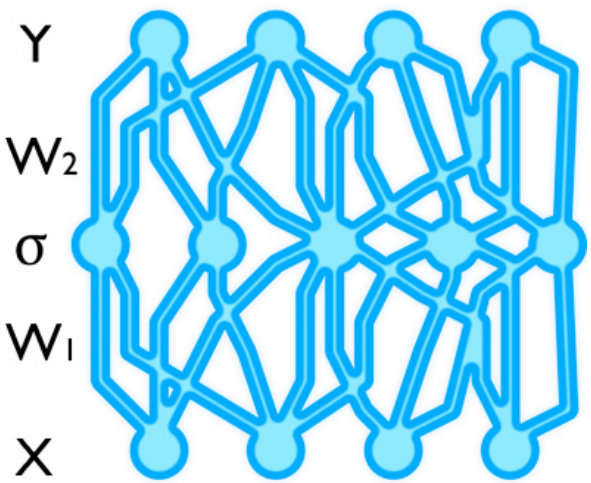

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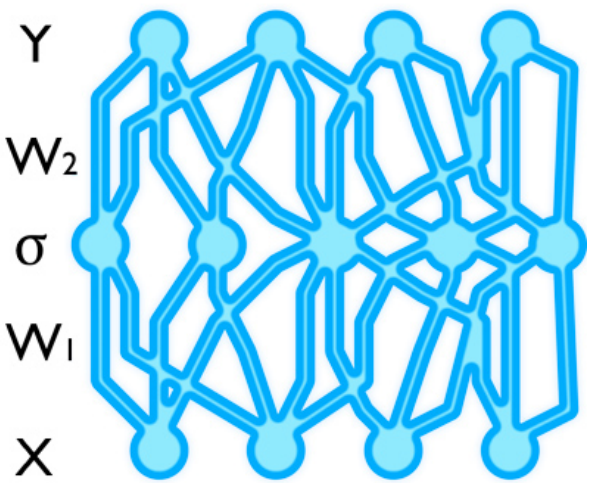

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- called "NNs" for historical reasons

- **layers**
  - ='feature vectors' in hierarchy
  - linear trans. = 'inner product' layer = 'fully connected' layer
  - 'input layer', 'output layer', 'hidden layers'
  - trans. matrix = weight matrix = W; intercept = bias = b

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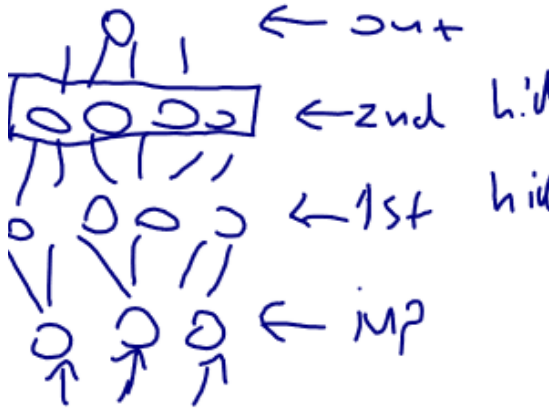

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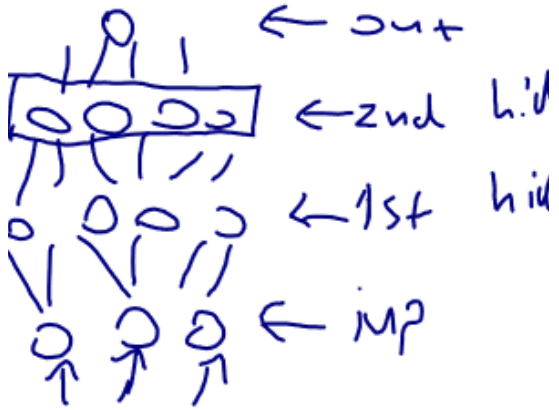

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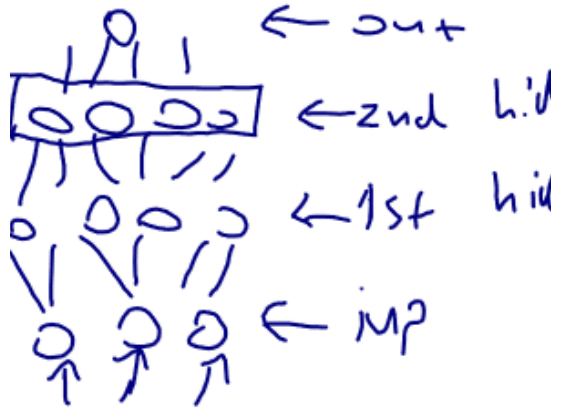

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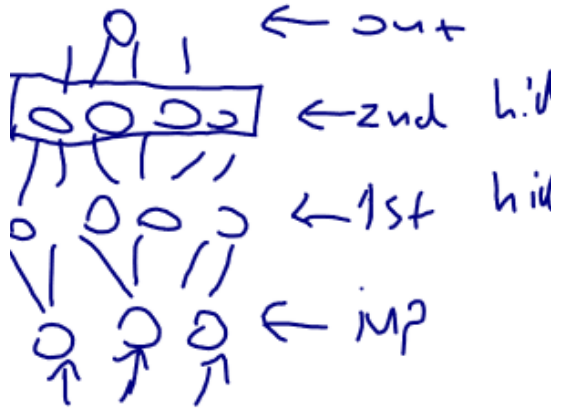
  - denote feature **vector** $\varphi(\mathbf{x}) = [\varphi_1(\mathbf{x}), .., \varphi_K(\mathbf{x})]$ with K units (a K by 1 vector)
  - denote feature **matrix** $\Phi = \varphi(\mathbf{X}) = [\varphi(\mathbf{x}_1)^T, ..., \varphi(\mathbf{x}_N)^T]$, N by K matrix (sometimes written $\Phi(\mathbf{X})$) [whiteboard]



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  - compose multiple basis function layers into a regression model
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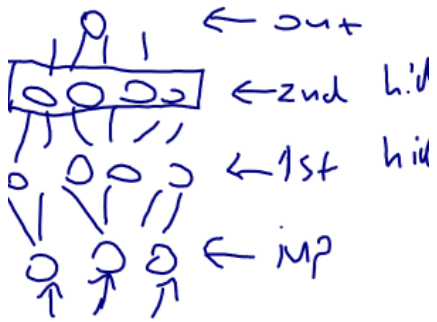

- classification
  - further compose a **softmax** function at the end; also called "logistic" for 2 classes
  - "squashes" its input → probability vector; prob vector also called model output / softmax vector / softmax layer

- "building blocks"
  - layers are simple
  - modularity in layer composition → versatility of deep models
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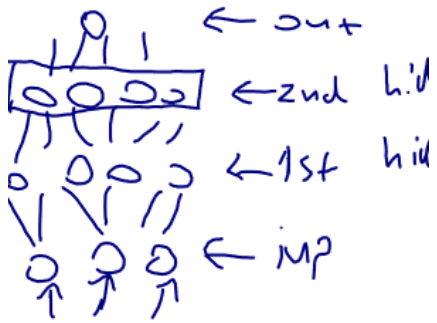

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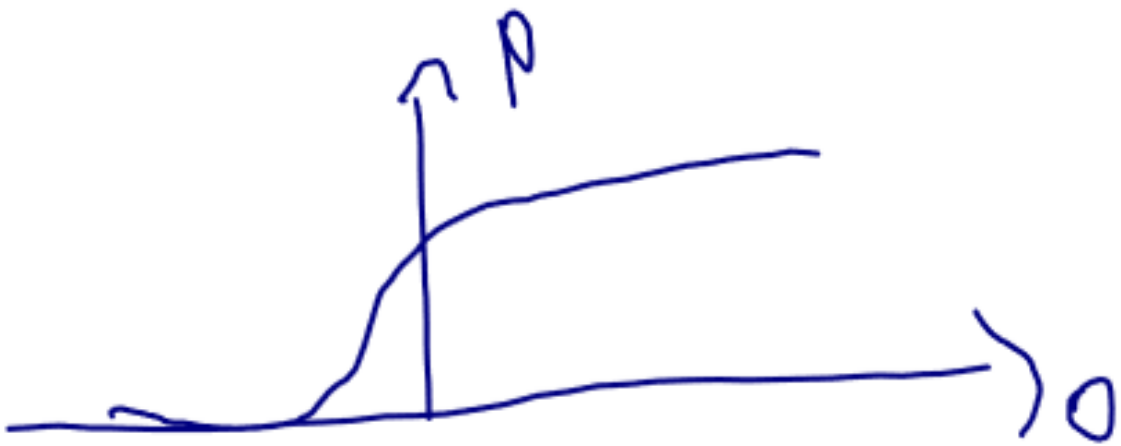

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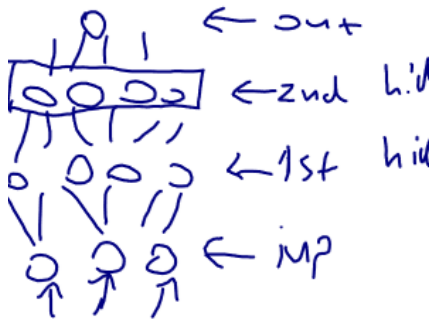

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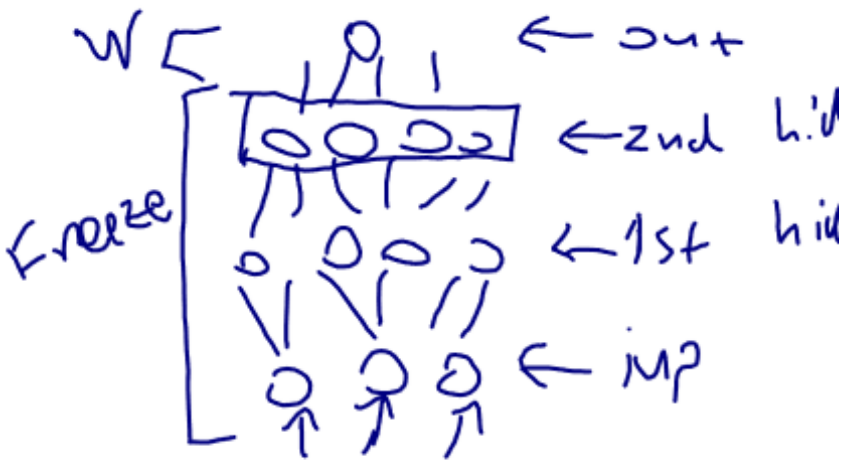

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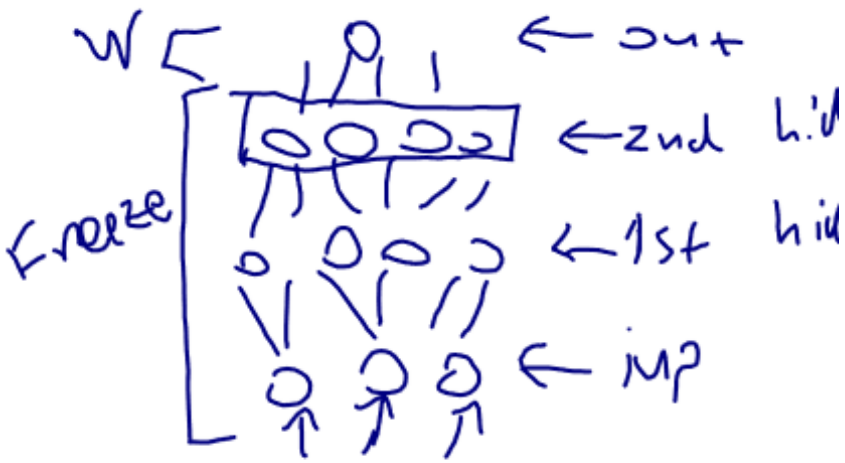

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Generative story

Want to put dist over functions..

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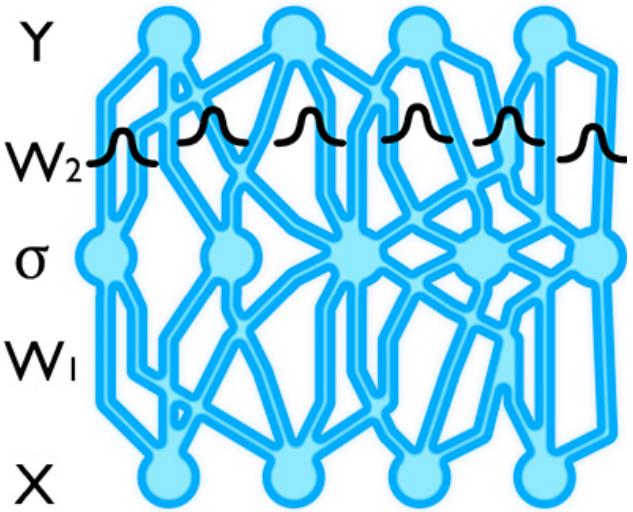

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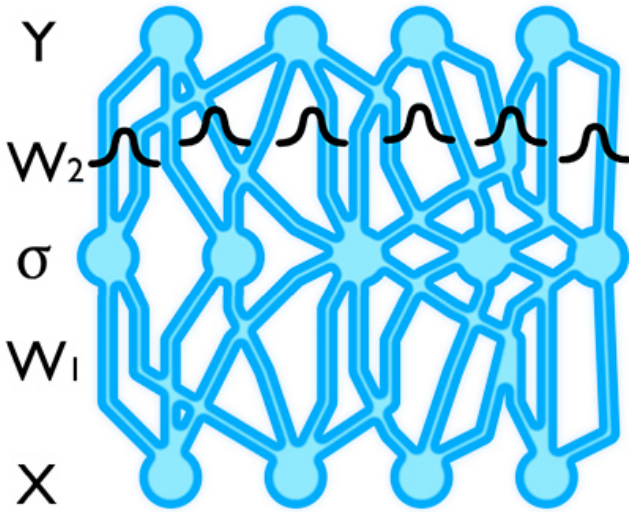

Generative story [what we assume about the data]

- Nature chose W which def's a func: $f^W(x) := W^T\varphi(x)$
- generated func. values with inputs $x_1, .., x_N$: $f^W(x_n)$
- ... and corrupted func. values with noise [also called "obs noise"] $y_n := f^W(x_n) + \epsilon_n,\ \epsilon_n \sim \mathcal{N}(0, \sigma^2)$ [additive Gaussian noise]
- we're given **observations** $\{(x_1, y_1), ..., (x_N, y_N)\}$ and $\sigma = 1$

Exercise: draw the graphical model (above fig is *information flow*, not graphical model)

Model

- qs
  - how can we find output y^* for a new x^*?
  - how can we find our confidence in this prediction?
  - $\rightarrow$ 'everything follows from the laws of probability theory'
- we build a **model**:
  - put prior dist over params W

$$p(w_k) = \mathcal{N}(w_k; 0, s^2) \qquad k \in [1, .., K]$$

  - likelihood [conditioned on W generate obs by adding gaussian noise]

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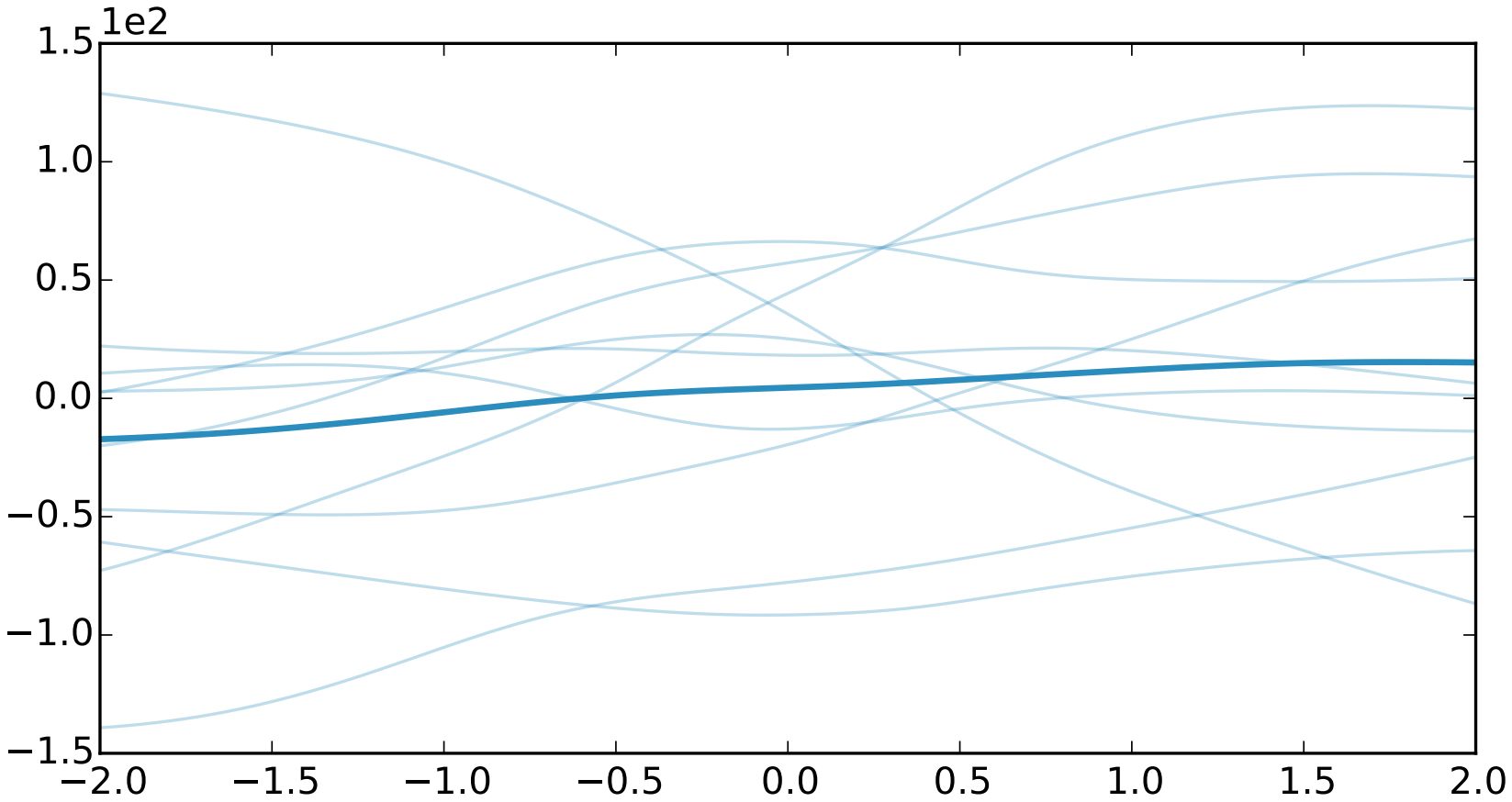
- prior belief "$w_k \sim \mathcal{N}(0, 1)$" means that **funcs** are likely to be smooth, vs "$w_k \in \mathcal{N}(0, 100)$" means funcs likely to be erratic; eg, visualising func draws from prior:



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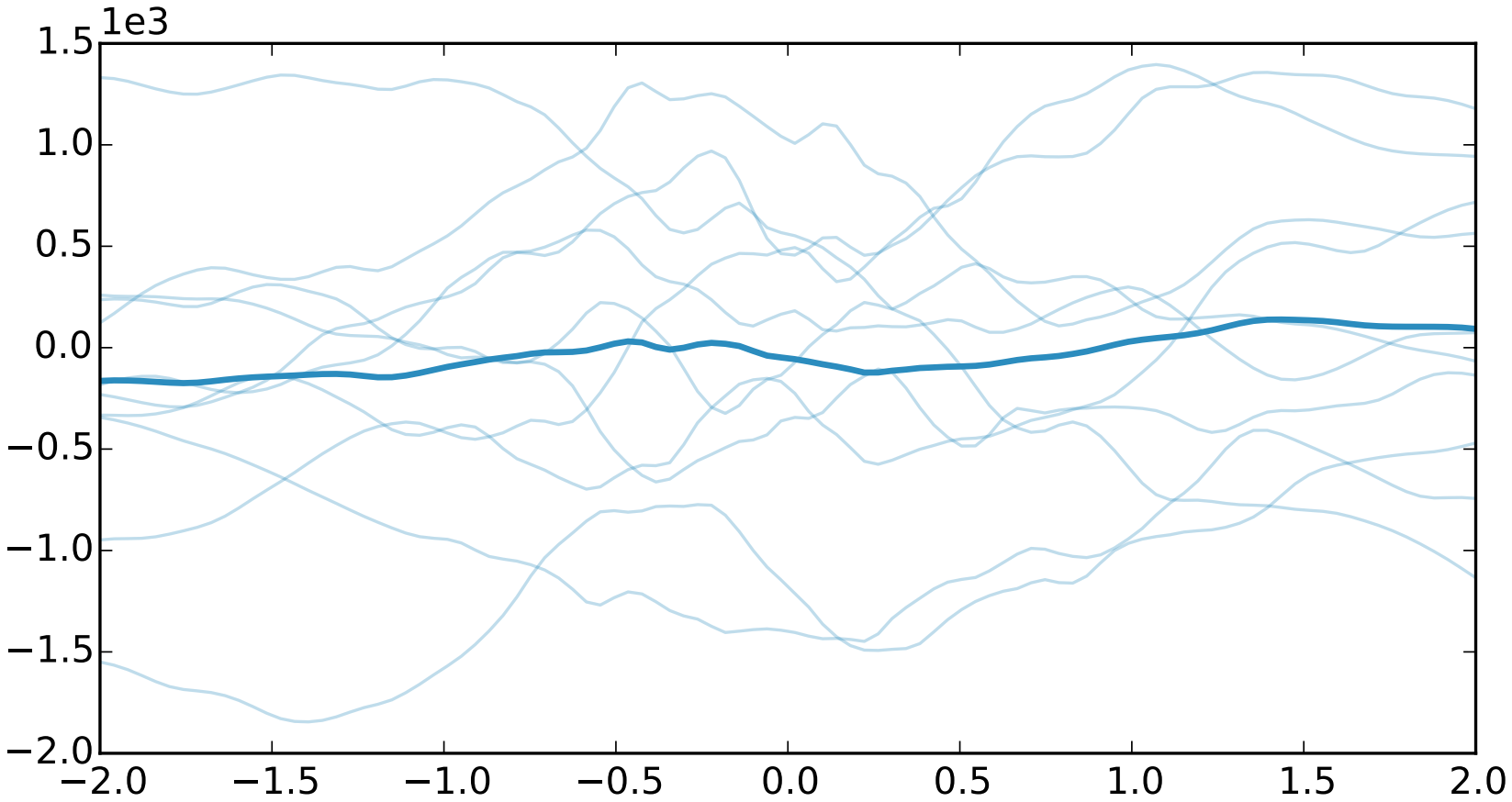

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To find a distribution over y^* for a new x^*

$$p(y^*|x^*, X, Y) \qquad \text{this is the } \textbf{predictive} \text{ dist (we'll use it a lot)}$$

$$= \int p(y^*, W|x^*, X, Y)\mathrm{d}W \qquad \text{sum rule}$$

$$= \int p(y^*|W, x^*, X, Y)p(W|x^*, X, Y)\mathrm{d}W \qquad \text{product rule}$$

$$= \int p(y^*|x^*, W)p(W|X, Y)\mathrm{d}W \qquad \text{model assumptions}$$

- we know the likelihood
- ... so we want to infer the posterior over W (find dist over W given $\mathcal{D}$)

Quick recap on Gaussians

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Products, ratios, marginals, and conditionals of Gaussians are Gaussian! (we'll use this a lot)

Properties of Gaussian distributions:

If x_1, x_2 follow a joint Gaussian distribution:

$$\begin{bmatrix} x_1, \\ x_2 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_1, \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12}^T & \Sigma_{22} \end{bmatrix} \right),$$

then each marginal is Gaussian:

$$x_1 \sim \mathcal{N}(\mu_1, \Sigma_{11}),$$

each conditional is Gaussian:

$$x_1 | x_2 \sim \mathcal{N}(\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2), \Sigma_{11} - \Sigma_{12}\Sigma_{22}\Sigma_{21}^T),$$

any linear combination is Gaussian:

$$Ax_1 + Bx_2 + C \sim \mathcal{N}(A\mu_1 + B\mu_2 + C, A\Sigma_{11}A^T + B\Sigma_{22}B^T)$$

and the product of the marginal densities is an (unnormalised) Gaussian:

$$\mathcal{N}(x; \mu_1, \Sigma_{11})\mathcal{N}(x; \mu_2, \Sigma_{22}) = C \cdot \mathcal{N}\left(x; (\Sigma_{11}^{-1} + \Sigma_{22}^{-1})^{-1}(\Sigma_{11}^{-1}\mu_1 + \Sigma_{22}^{-1}\mu_2), (\Sigma_{11}^{-1} + \Sigma_{22}^{-1})^{-1}\right)$$

with $C = \mathcal{N}(\mu_1; \mu_2, \Sigma_{11} + \Sigma_{22})$.

More here.

Visualising Gaussian likelihoods:

Summary (and playgroud) here: yr.gl/udl101

Analytic inference w functions [new technique!]

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Claim: if the prior and likelihood are Gaussians, then the posterior prob over W must be Gaussian too (this is called *conjugacy*).

- Exercise

Analytic inference w functions [new technique!]

Claim: if the prior and likelihood are Gaussians, then the posterior prob over W must be Gaussian too (this is called *conjugacy*).

- Exercise

We've shown the posterior is Gaussian. Therefore we can write it as $\mathcal{N}(W; \mu', \Sigma')$.
Write

$$p(W|X, Y) = \mathcal{N}(W; \mu', \Sigma')$$

and expand both sides to find μ', Σ':

$$p(w|x,y) = p(y|x,w)\,p(w|x)\,/\,p(y|x)$$

[whiteboard]

we're basically 'completing the squares' in the exponents.

Analytic inference w functions [new technique!]

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- posterior variance

$$\Sigma' = (\sigma^{-2} \sum_n (\varphi(x_n)\varphi(x_n)^T) + s^{-2} I_K)^{-1}$$

and in vector form: $(\sigma^{-2}\Phi(\mathbf{X})^T\Phi(\mathbf{X}) + s^{-2} I_K)^{-1}$

- posterior mean

$$\mu' = \Sigma'\sigma^{-2} \sum_n (y_n \varphi(x_n))$$

and in vector form: $\Sigma'\sigma^{-2}\Phi(\mathbf{X})^T\mathbf{Y}$

Exercise: show that $\sum_n (\varphi(x_n)\varphi(x_n)^T) = \Phi(\mathbf{X})^T\Phi(\mathbf{X})$ and $\sum_n (y_n\varphi(x_n)) = \Phi(\mathbf{X})^T\mathbf{Y}$.

Analytic predictions with functions

Coming back to predicting function values y^* for new x^*

- There's only one correct way – use prob theory to perform preds!

$$p(y^*|x^*, X, Y) \qquad \text{this is the } \textbf{predictive} \text{ dist (we'll use it a lot)}$$

$$= \int p(y^*, W|x^*, X, Y)\mathrm{d}W \qquad \text{sum rule}$$

$$= \int p(y^*|W, x^*, X, Y)p(W|x^*, X, Y)\mathrm{d}W \qquad \text{product rule}$$

$$= \int p(y^*|x^*, W)p(W|X, Y)\mathrm{d}W \qquad \text{model assumptions}$$

- how to eval? [a new technique!]
  - likelihood $p(y^*|x^*, W)$ is Gaussian
  - posterior $p(W|X, Y)$ is Gaussian (from above)
  - so joint $p(y^*, W|x^*, X, Y)$ is Gaussian (conjugacy)
  - and *predictive* $p(y^*|x^*, X, Y)$ is Gaussian (marginal)

Analytic predictions with functions

We know that the likelihood and posterior are Gaussians, therefore the predictive prob over y^* must be Gaussian too (conjugacy). We'll use moment matching to find it:

$$p(y^* | x^*, \mathcal{D}) = \mathcal{N}(\mu^*, \Sigma^*)$$

$$\mu^* = \mathbb{E}_{p(y^*|x^*,\mathcal{D})}[y^*]$$

[whiteboard]

Analytic predictions with functions

We know that the likelihood and posterior are Gaussians, therefore the predictive prob over y^* must be Gaussian too (conjugacy). We'll use moment matching to find it:

$$p(y^*|x^*, \mathcal{D}) = \mathcal{N}(\mu^*, \Sigma^*)$$

$$\mu^* = \mathbb{E}_{p(y^*|x^*,\mathcal{D})}[y^*]$$

$$\ldots = \mu'^T \varphi(x^*)$$

- **Exercise** (10min): Derive the variance of the predictive distribution (predictive variance) (hint: use the identity $Var(z) = E[z^T z] - E[z]^T E[z]$ with simple manipulations)

Useful resources: yr.gl/udl101

Analytic predictions with functions (Exercise)

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- Predictive variance (hint: use the identity $Var(z) = E[z^T z] - E[z]^T E[z]$ with simple manipulations)

$$E(y^*) = \mu'^T \varphi(x^*)$$
$$\text{var}(y^*) = E_{p(y^*|\ldots)}[y^{*T} y^*] - \mu^{*T} \mu^* = \sigma^2 + \varphi(x^*)^T \Sigma' \varphi(x^*)$$

Questions & discussion