



UNIVERSITY OF  
CAMBRIDGE

# Quantification of Beliefs

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<http://carlhenrik.com>

Me

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- Lecturer in Machine Learning
- Bayesian non-parametrics
- Vehicle Engineer by Training





# Today

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- Why are uncertainties not just desirable but necessary for learning

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- Why knowledge is subjective or relative

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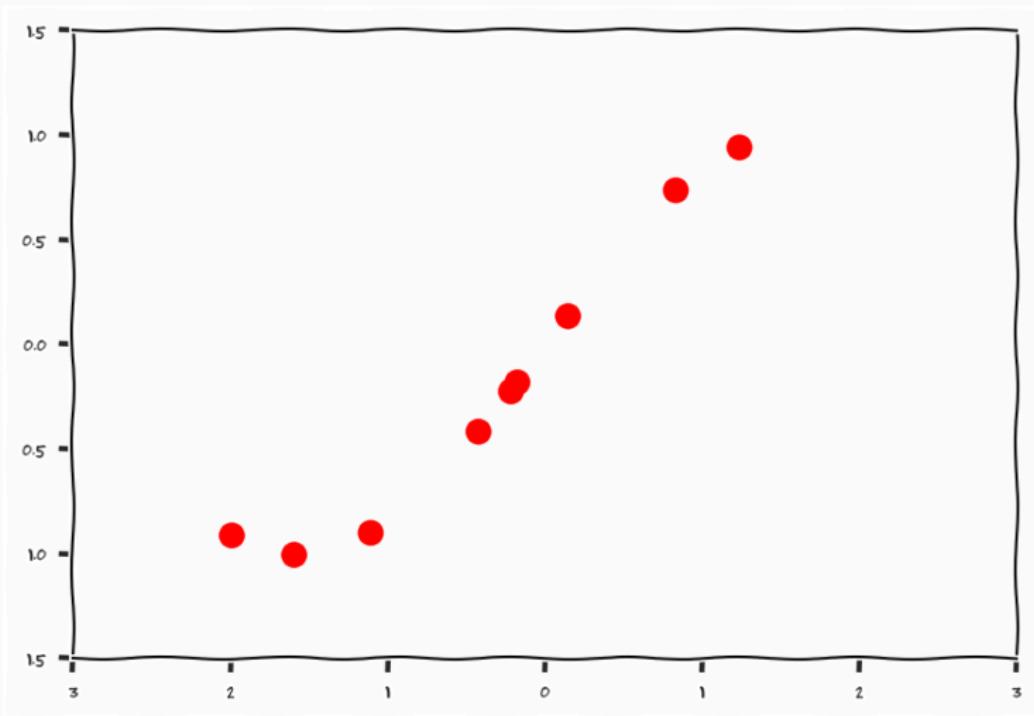
- Why are uncertainties not just desirable but necessary for learning
- Why knowledge is subjective or relative
- Re-cap of linear regression

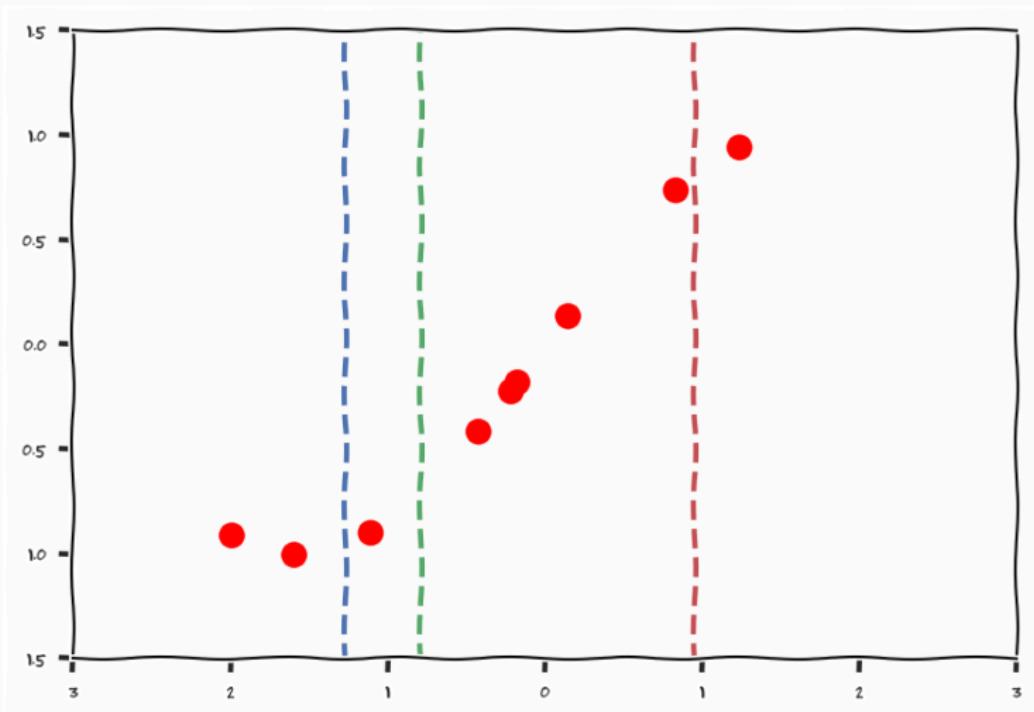
# Inductive Reasoning

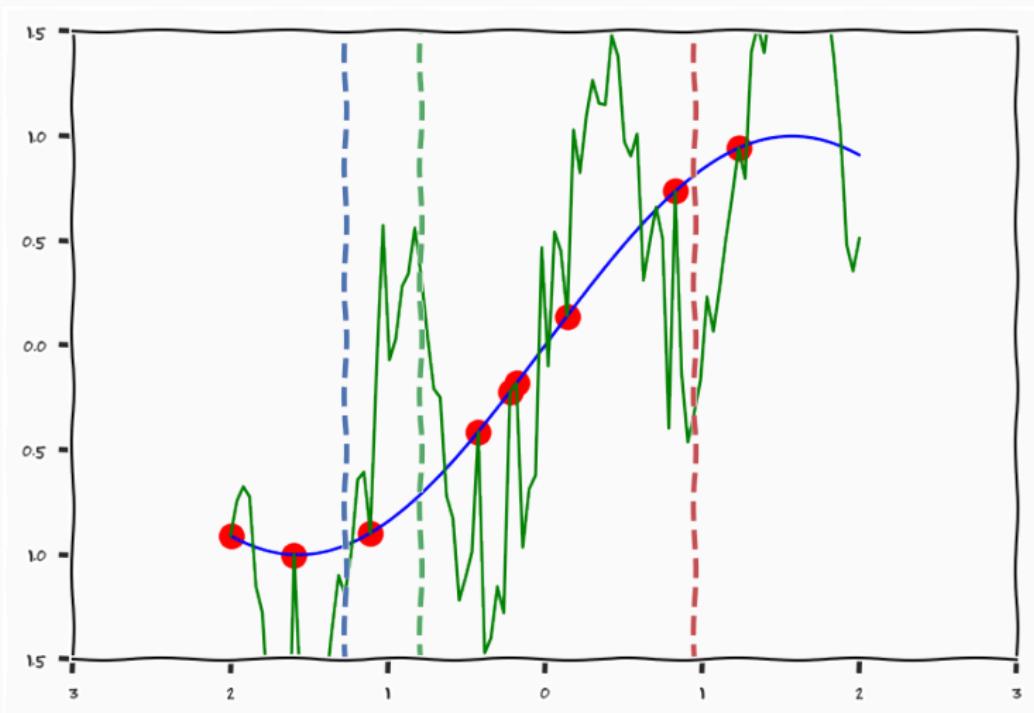
## Inductive Reasoning

"In inductive inference, we go from the specific to the general. We make many observations, discern a pattern, make a generalization, and infer an explanation or a theory"

– Wassertheil-Smoller





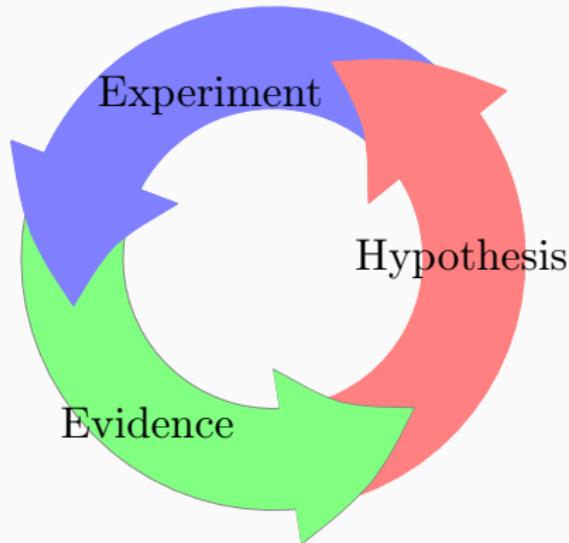


# Inductive Reasoning II

## Inductive Reasoning

Unlike deductive arguments, inductive reasoning allows for the possibility that the conclusion is false, even if all of the premises are true.

# The Scientific Principle



$$\text{Data} + \text{Model} \xrightarrow{\text{Compute}} \text{Prediction}$$

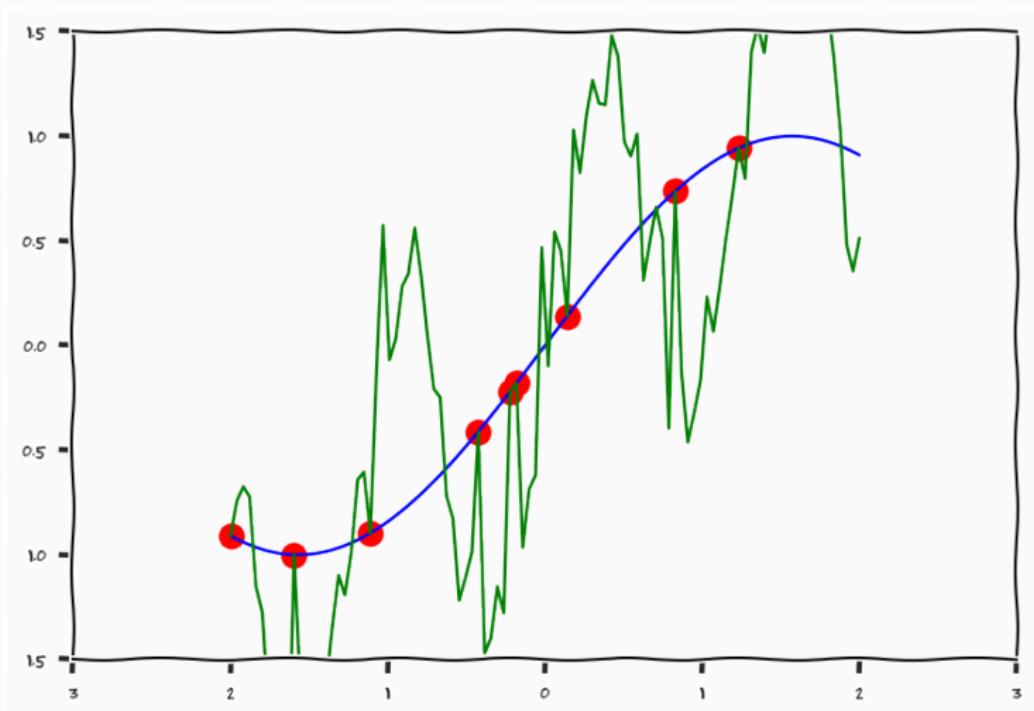
## "The Machine Learning Principle"<sup>1</sup>

*"There is a notion of success . . . which I think is novel in the history of science. It interprets success as approximating unanalyzed data."*

*– Prof. Noam Chomsky*

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<sup>1</sup>Chomsky et al., 1980



# Learning Theory

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- $\mathcal{F}$  space of functions

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- $\mathcal{F}$  space of functions
- $\mathcal{A}$  learning algorithm

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# Learning Theory

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- $\mathcal{F}$  space of functions
- $\mathcal{A}$  learning algorithm
- $\mathcal{S} \sim P(\mathcal{X} \times \mathcal{Y})$
- $\mathcal{S} = \{(x_1, y_1), \dots, (x_N, y_N)\}$
- $\ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y)$  loss function

$$e(\mathcal{S}, \mathcal{A}, \mathcal{F}) = \mathbb{E}_{P(\{\mathcal{X}, \mathcal{Y}\})} [\ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y)]$$

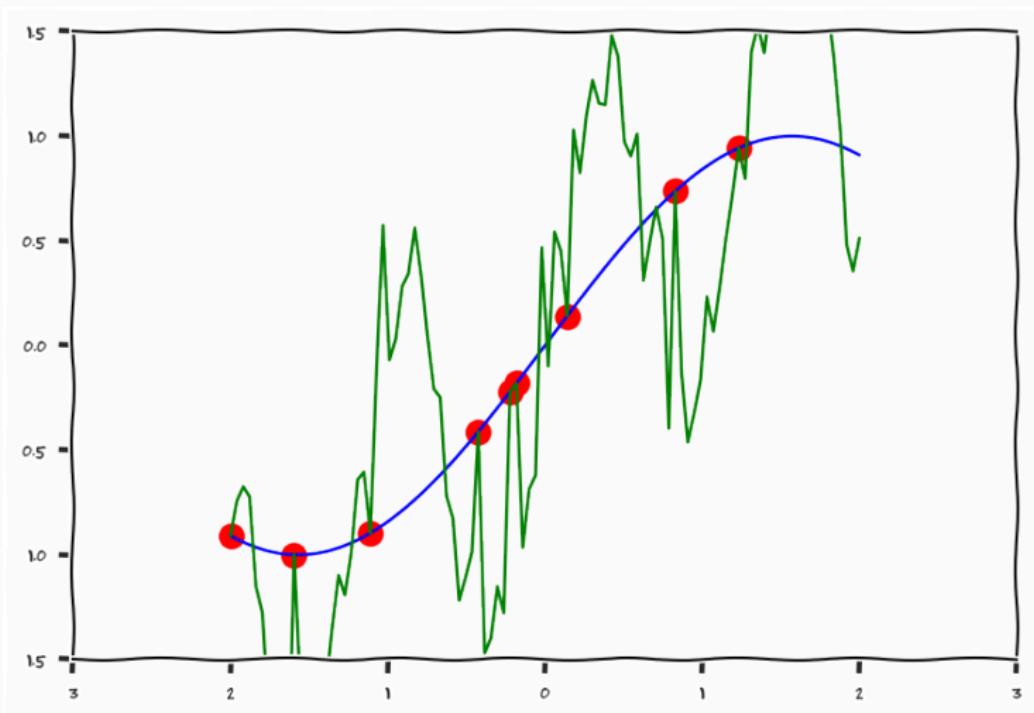
$$\begin{aligned} e(\mathcal{S}, \mathcal{A}, \mathcal{F}) &= \mathbb{E}_{P(\{\mathcal{X}, \mathcal{Y}\})} [\ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y)] \\ &= \int \ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y) p(x, y) dx dy \end{aligned}$$

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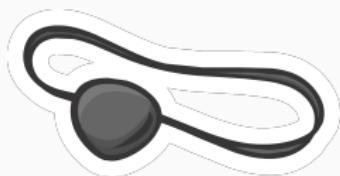
## No Free Lunch

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We can come up with a combination of  $\{\mathcal{S}, \mathcal{A}, \mathcal{F}\}$  that makes  $e(\mathcal{S}, \mathcal{A}, \mathcal{F})$  take an arbitrary value



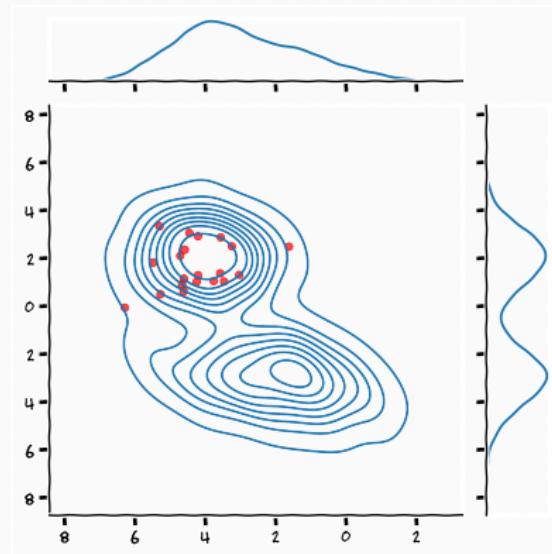
## Assumptions: Algorithms



Statistical Learning

$$\mathcal{A}_{\mathcal{F}}(\mathcal{S})$$

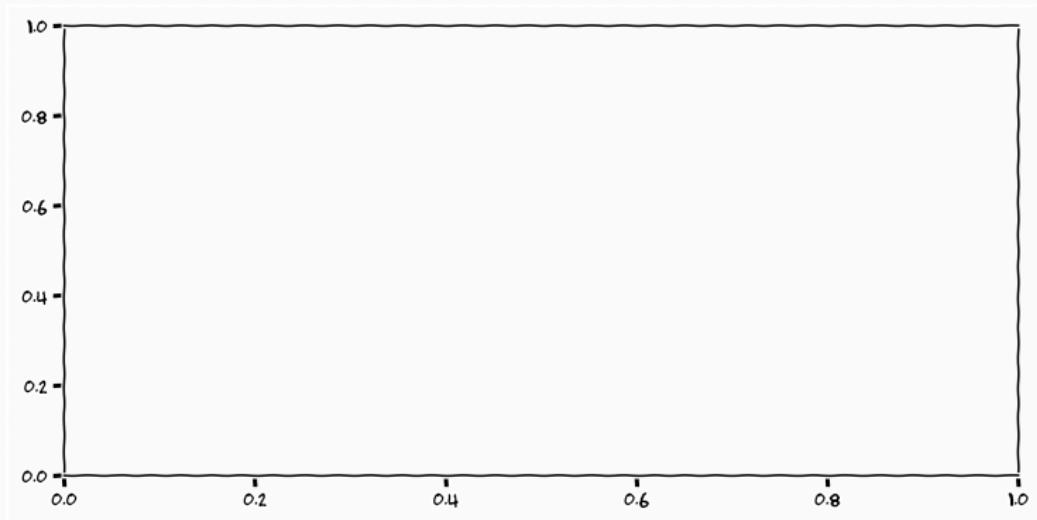
## Assumptions: Biased Sample



Statistical Learning

$$\mathcal{A}_{\mathcal{F}}(\mathcal{S})$$

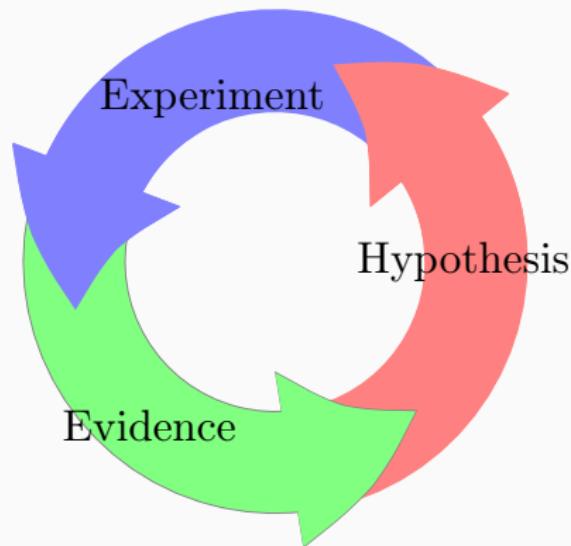
## Assumptions: Hypothesis space



Statistical Learning

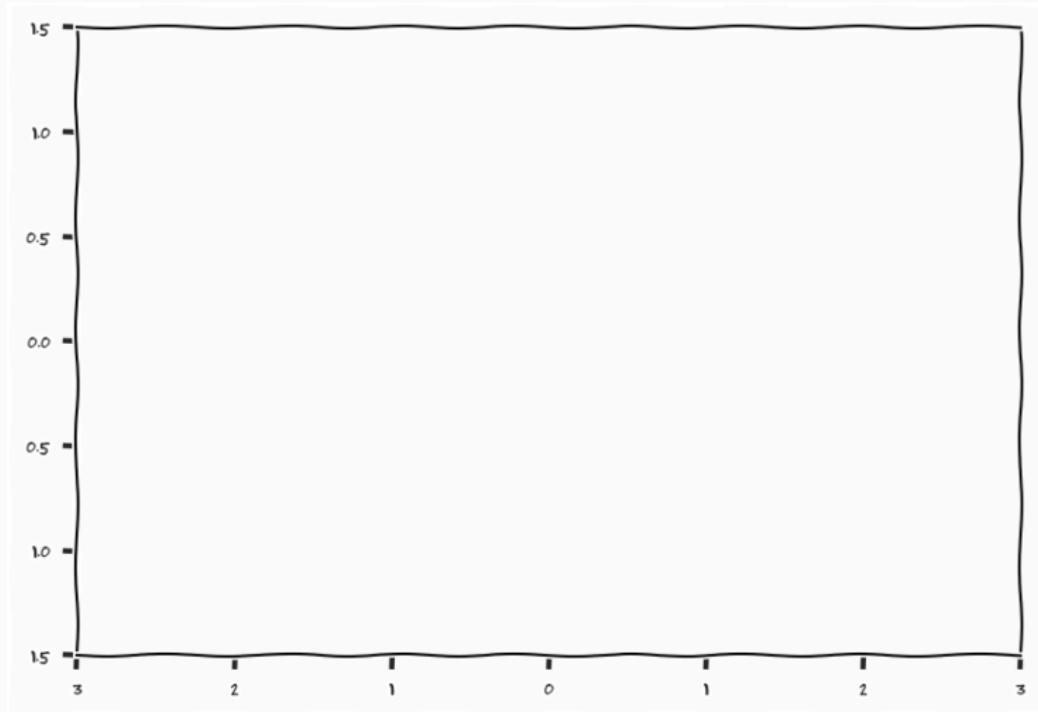
$$\mathcal{A}_{\mathcal{F}}(\mathcal{S})$$

# The Scientific Principle

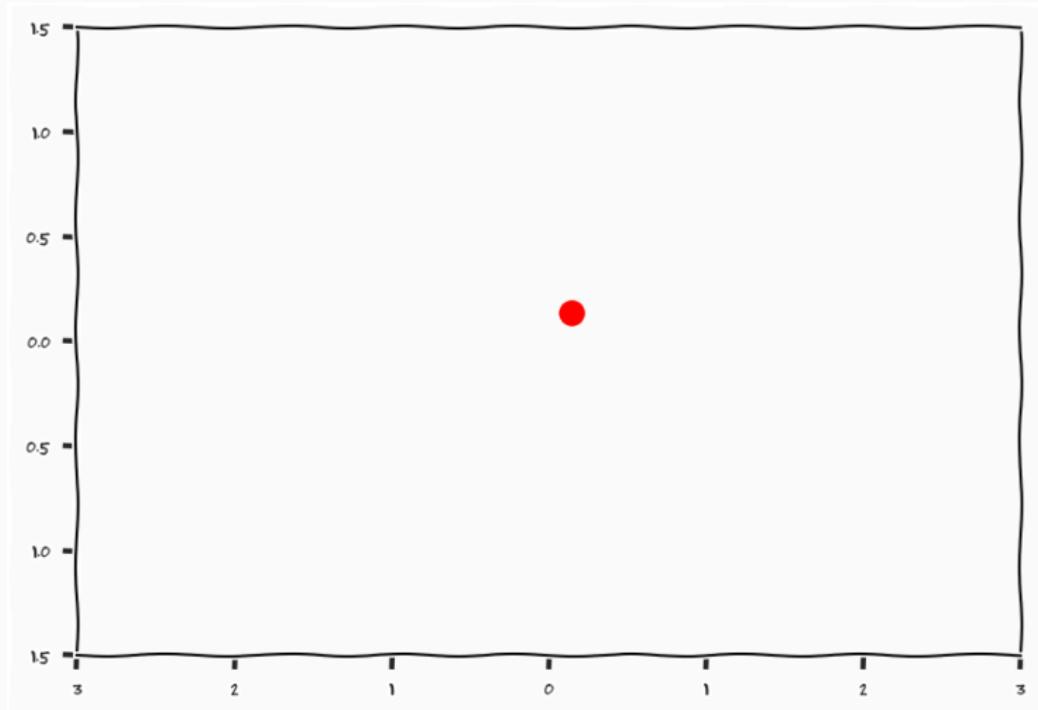


$$\text{Data} + \text{Model} \xrightarrow{\text{Compute}} \text{Prediction}$$

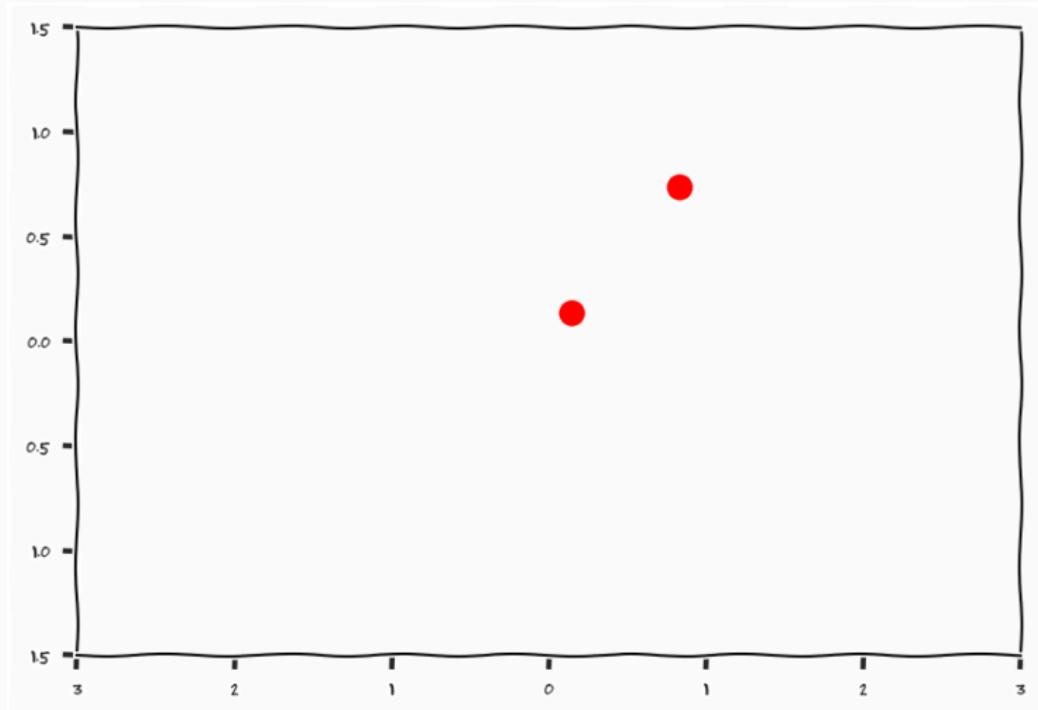
## Example



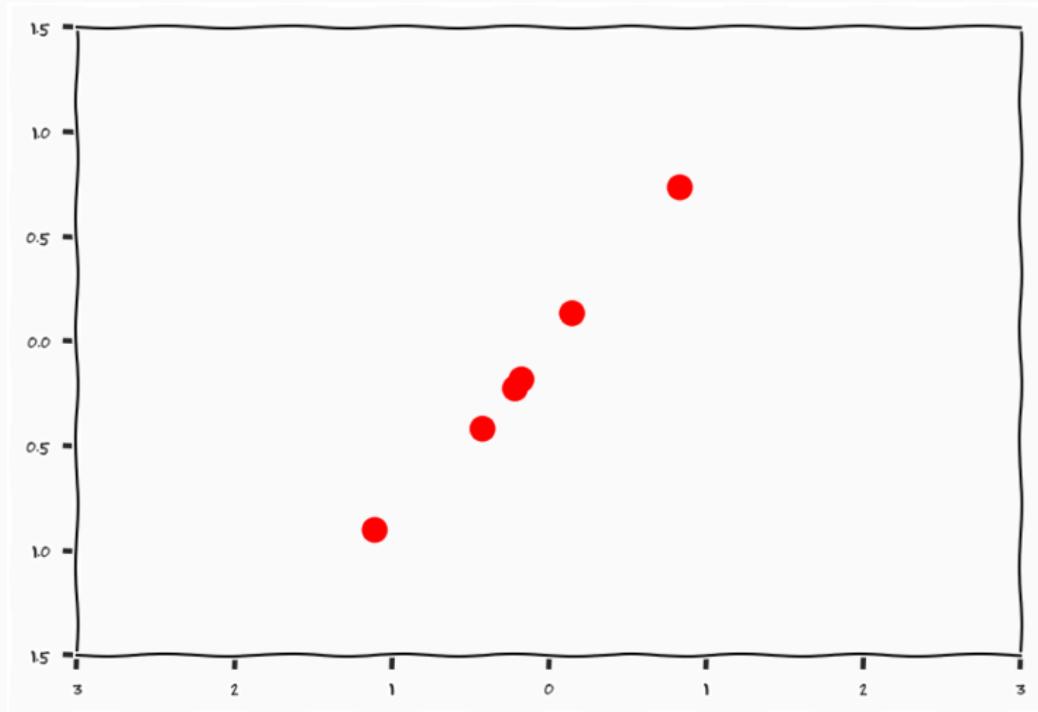
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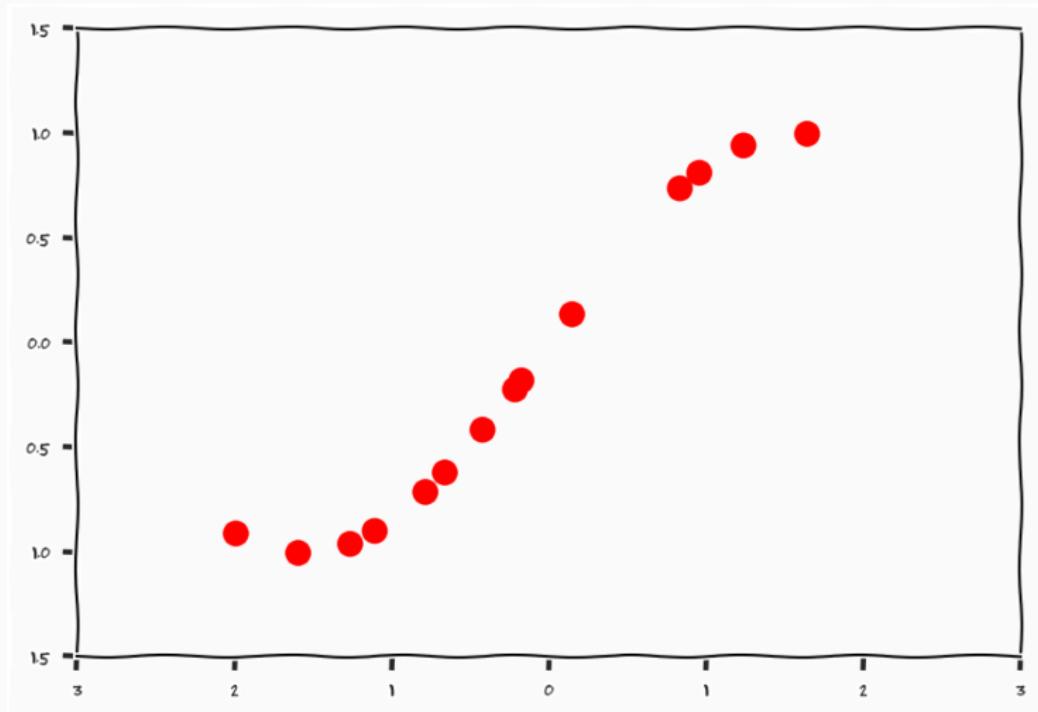
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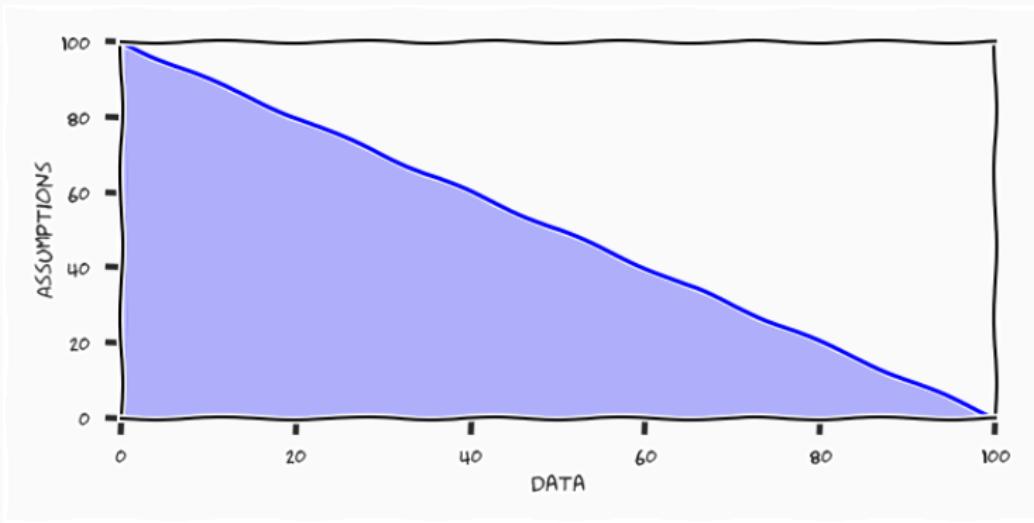
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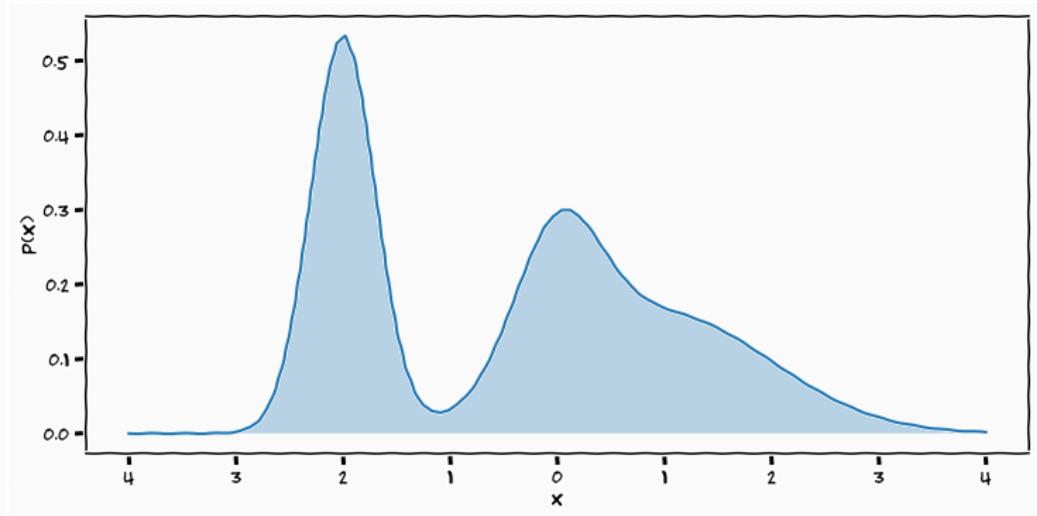
## Example



# Data and Beliefs



# Encoding Beliefs



# Manipulation of Beliefs

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Sum Rule

$$p(y) = \sum p(y, \theta)$$

Product Rule

$$p(y, \theta) = p(y \mid \theta)p(\theta)$$

## Laplace Laplace, 1814



"On voit, par cet Essai, que la théorie des probabilités n'est, au fond, que le bon sens réduit au calcul; elle fait apprécier avec exactitude ce que les esprits justes sentent par une sorte d'instinct, sans qu'ils puissent souvent s'en rendre compte."

– Simon Laplace

## Laplace Laplace, 1814



"One sees, from this Essay, that the theory of probabilities is basically just common sense reduced to calculus; it makes one appreciate with exactness that which accurate minds feel with a sort of instinct, often without being able to account for it."

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## Baye's "Rule"

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$$p(y, \theta) = p(y|\theta)p(\theta)$$

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$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$$

$$= \frac{p(y|\theta)p(\theta)}{\sum p(y|\theta)p(\theta)}$$

$$p(\theta | y) = \frac{p(y | \theta)p(\theta)}{\int p(y | \theta)p(\theta)d\theta}$$

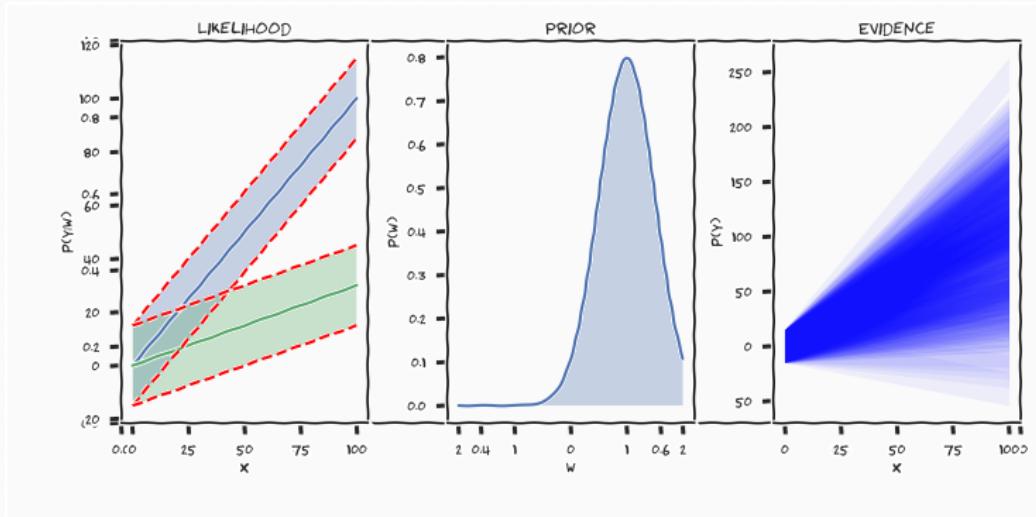
**Likelihood** How much **evidence** is there in the data for a specific hypothesis

**Prior** What are my beliefs about different hypothesis

**Posterior** What is my **updated** belief after having seen data

**Evidence** What is my belief about the data

# Regression Model



$$y = x \cdot w \pm 15$$

$$w \sim \mathcal{N}(1, 0.5)$$

# Uncertainty

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**Data** Today

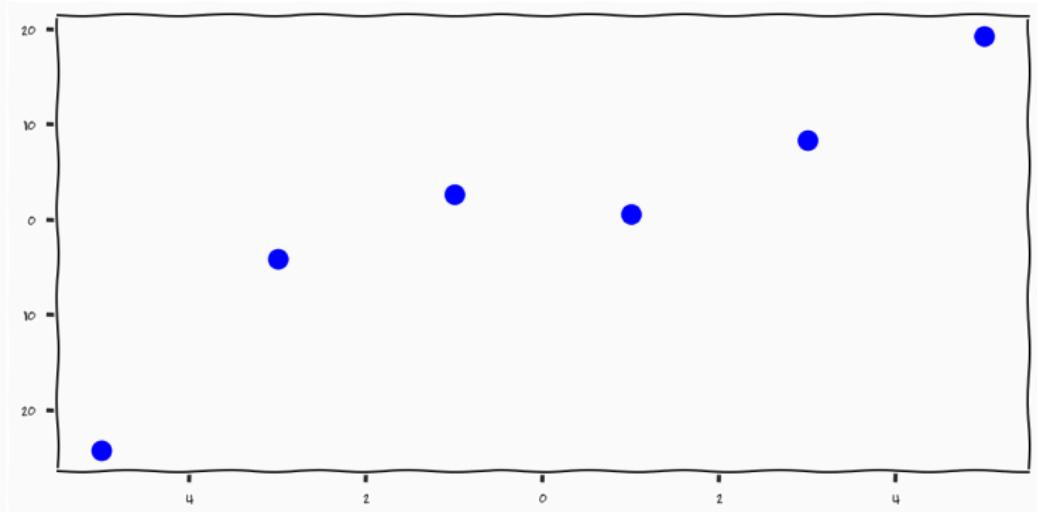
**Model** Thursday

**Computation** Friday

# Linear Regression

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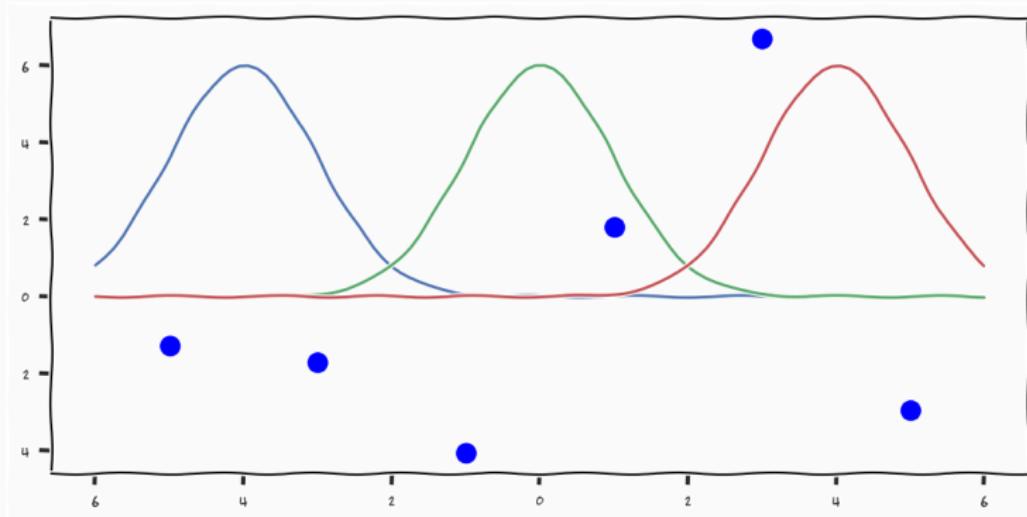
# Linear Regression



- Linear function in both parameters and data

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \dots + w_D x_D = \mathbf{w}^T \mathbf{x} + w_0 = \{D = 1\} w_0 + w_1 * x$$

# Linear Regression



- Linear function only in parameters

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$$

# Linear Regression

---

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}^T \begin{bmatrix} 1 \\ x \end{bmatrix}$$

- Given observations of data pairs  $\mathcal{D} = \{y_i, \mathbf{x}_i\}_{i=1}^N$  can we infer what  $\mathbf{w}$  should be

# Linear Regression

---

Task 1 define a likelihood (**model**)

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- what output do I consider likely under a given hypothesis?

# Linear Regression

---

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**Task 2** define an assumption/belief over all hypothesis  
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- what types of models do I think are more probable than others

**Task 3** update my belief with new observations (**data**)

- formulate posterior (**compute**)

**Task 4** predict using my new belief (**predict**)

- formulate predictive distribution

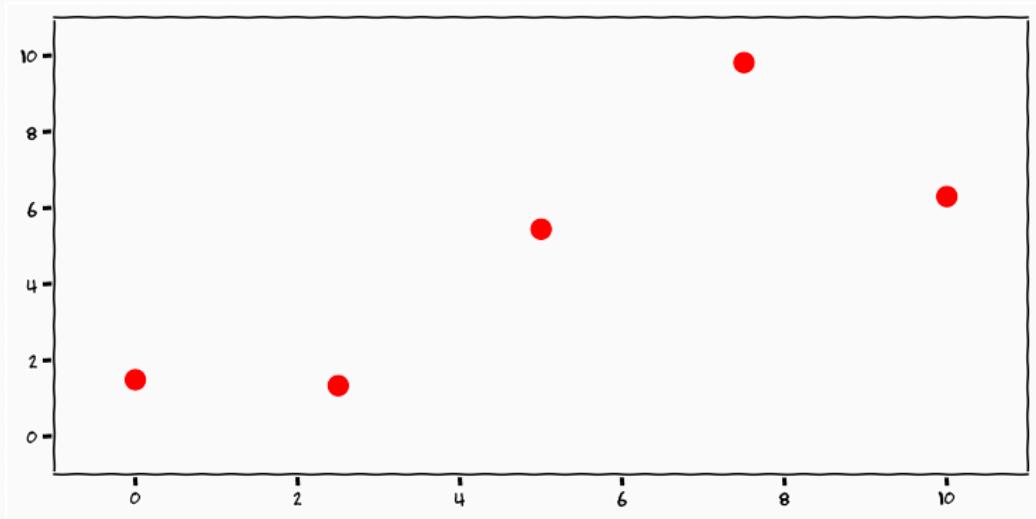
## Linear Regression

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$$\begin{aligned}y &= f(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^T \mathbf{x} + \epsilon \\ \epsilon &\sim \mathcal{N}(0, \beta^{-1} I)\end{aligned}$$

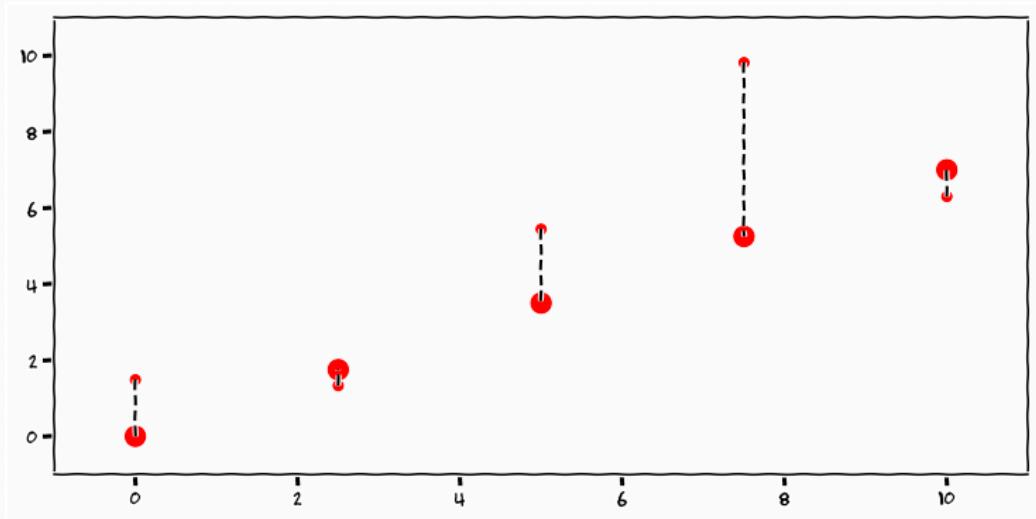
- We assume that we have been given data pairs  $\{y_i, \mathbf{x}_i\}_{i=1}^N$  corrupted by additive noise
- We assume that the distribution of the noise follows a Gaussian

# Explaining Away



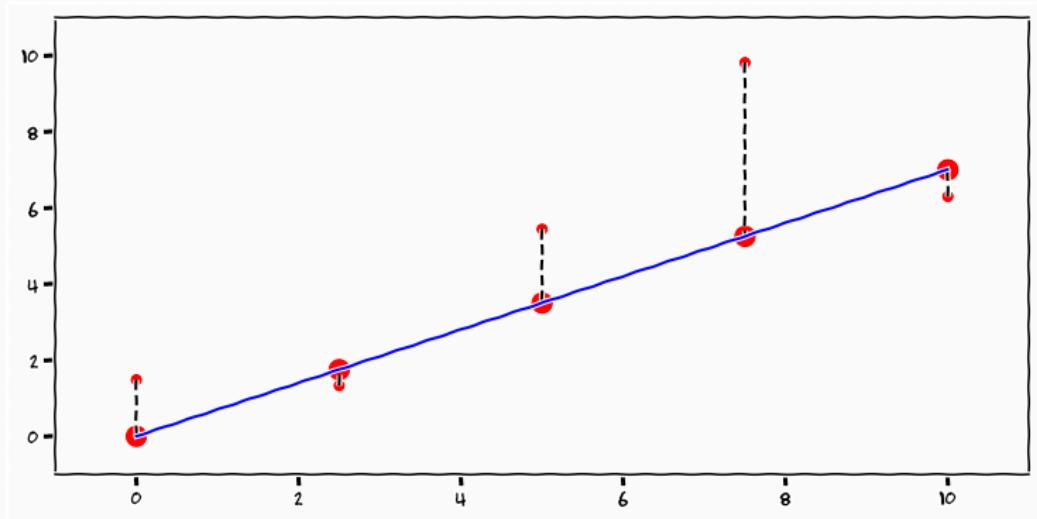
$$y = \mathbf{w}^T x + \epsilon$$

# Explaining Away



$$y - \epsilon = \mathbf{w}^T x$$

# Explaining Away



$$\tilde{y} = \mathbf{w}^T x$$

# Likelihood

---

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---

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$$y = \mathbf{w}^T \mathbf{x} + \epsilon$$

$$y - \mathbf{w}^T \mathbf{x} = \epsilon$$

$$y - \mathbf{w}^T \mathbf{x} \sim \mathcal{N}(\epsilon | 0, \beta^{-1} I) = \left( \frac{\beta}{2\pi} \right)^{\frac{1}{2}} e^{-\frac{1}{2}(\epsilon-0)\beta(\epsilon-0)}$$

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$$\Rightarrow \mathcal{N}(y - \mathbf{w}^T \mathbf{x} | 0, \beta^{-1} I) = \left( \frac{\beta}{2\pi} \right)^{\frac{1}{2}} e^{-\frac{1}{2}(y - \mathbf{w}^T \mathbf{x})\beta(y - \mathbf{w}^T \mathbf{x})}$$

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$$\Rightarrow \mathcal{N}(y - \mathbf{w}^T \mathbf{x} | 0, \beta^{-1} I) = \mathcal{N}(y | \mathbf{w}^T \mathbf{x}, \beta^{-1} I)$$

$$\Rightarrow p(y | \mathbf{w}, \mathbf{x}) = \mathcal{N}(y | \mathbf{w}^T \mathbf{x}, \beta^{-1} I)$$

# Likelihood

- Likelihood

$$p(y|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(y|\mathbf{w}^T \mathbf{x}, \beta^{-1})$$

- Independence

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^N \mathcal{N}(y_n|\mathbf{w}^T \mathbf{x}_n, \beta^{-1})$$

Assume each output to be independent given the input and the parameters

# Linear Regression

---

- Likelihood is Gaussian in  $\mathbf{w}$

$$p(y|\mathbf{w}, \mathbf{x}) = \mathcal{N}(y|\mathbf{w}^T \mathbf{x}, \beta^{-1} I)$$

# Linear Regression

---

- Likelihood is Gaussian in  $\mathbf{w}$

$$p(y|\mathbf{w}, \mathbf{x}) = \mathcal{N}(y|\mathbf{w}^T \mathbf{x}, \beta^{-1} I)$$

- Conjugate Prior

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$$

# Linear Regression

---

- Likelihood is Gaussian in  $\mathbf{w}$

$$p(y|\mathbf{w}, \mathbf{x}) = \mathcal{N}(y|\mathbf{w}^T \mathbf{x}, \beta^{-1} I)$$

- Conjugate Prior

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$$

- Posterior

$$p(\mathbf{w}|\mathbf{y}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

# Linear Regression

- Likelihood is Gaussian in  $\mathbf{w}$

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# Linear Regression

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- $\mathbf{m}_N, \mathbf{S}_N$  is the mean and the co-variance of the posterior after having seen  $N$  data-points
- Gaussian identities

- Posterior is Gaussian

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

## Posterior

---

- Posterior is Gaussian

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

- Identification

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) \propto p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

# Posterior

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- Posterior is Gaussian

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

- Identification

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) \propto p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

- Posterior

$$\mathbf{m}_N = (\mathbf{S}_0^{-1} + \beta \mathbf{X}^T \mathbf{X})^{-1} (S_0^{-1} \mathbf{m}_0 + \beta \mathbf{X}^T \mathbf{y})$$

$$\mathbf{S}_N = (\mathbf{S}_0^{-1} + \beta \mathbf{X}^T \mathbf{X})^{-1}$$

## Posterior

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- Assumption Zero mean isotropic Gaussian

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|0, \alpha^{-1}\mathbf{I})$$

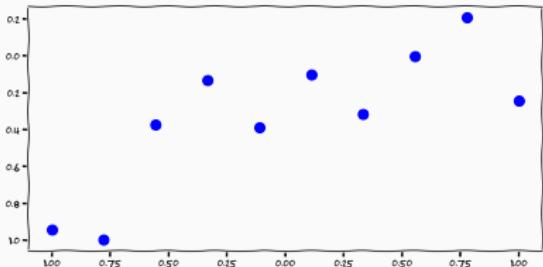
- Assumption Zero mean isotropic Gaussian

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|0, \alpha^{-1}\mathbf{I})$$

- Posterior

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\beta (\alpha\mathbf{I} + \beta\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}, (\alpha\mathbf{I} + \beta\mathbf{X}^T\mathbf{X})^{-1})$$

# Linear Regression Example



- Model

$$f(x, \mathbf{w}) = w_0 + w_1 x$$

- Data

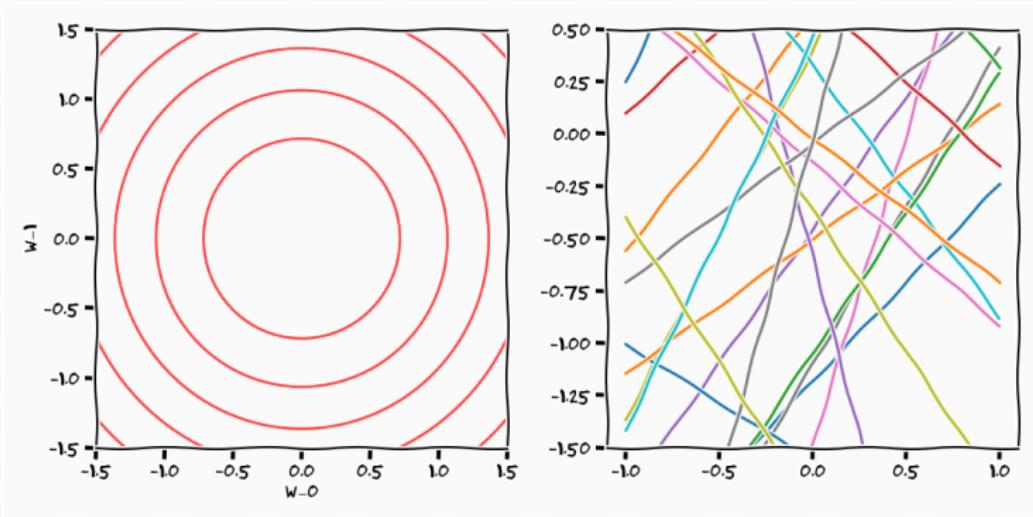
$$f(x, \mathbf{a}) = a_0 + a_1 x, \quad \{a_0, a_1\} = \{-0.3, 0.5\}$$

$$y = f(x, \mathbf{a}) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 0.2^2)$$

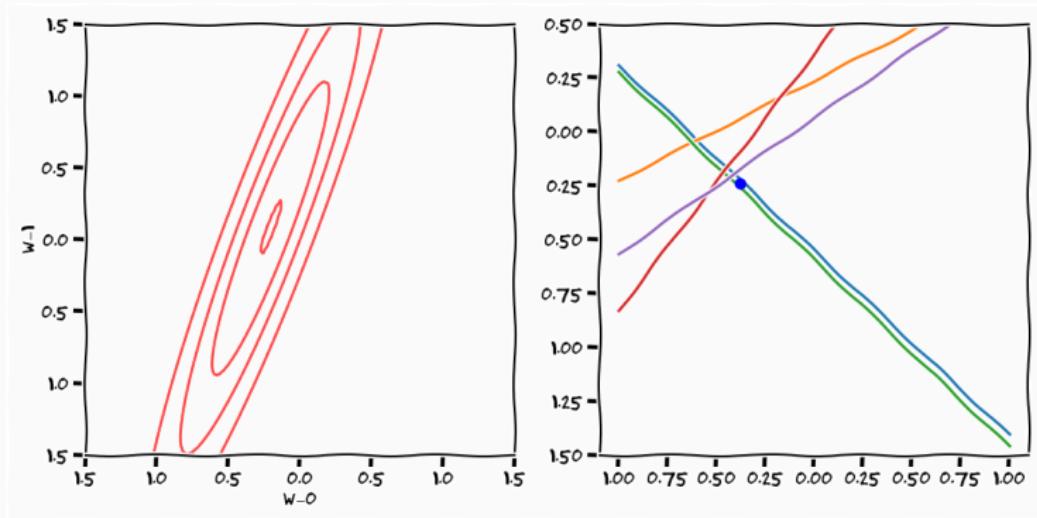
- Prior

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{0}, 2.0 \cdot \mathbf{I})$$

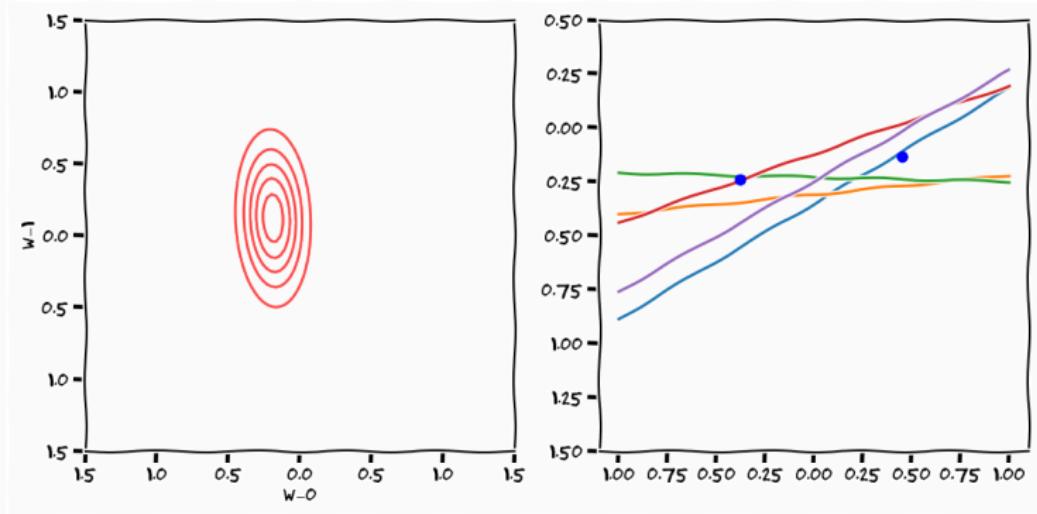
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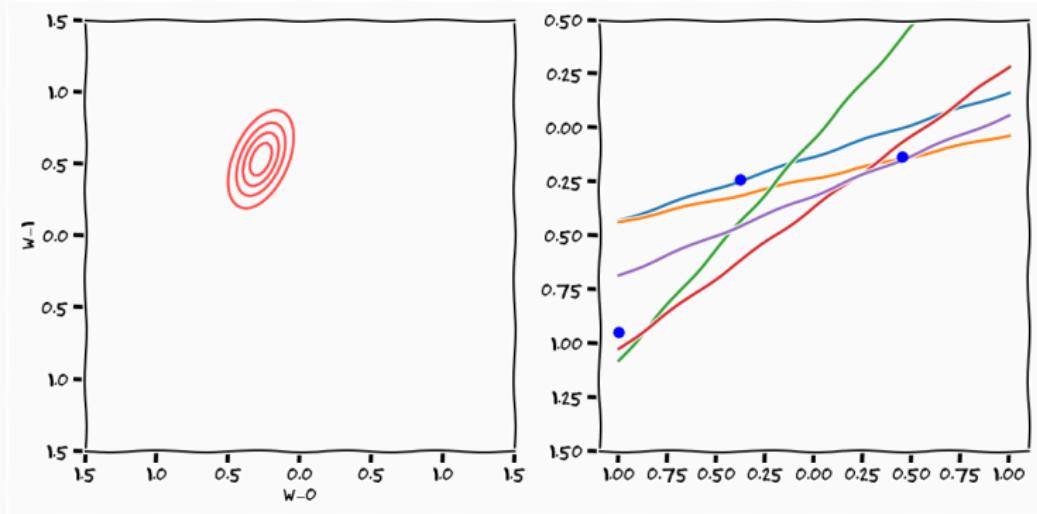
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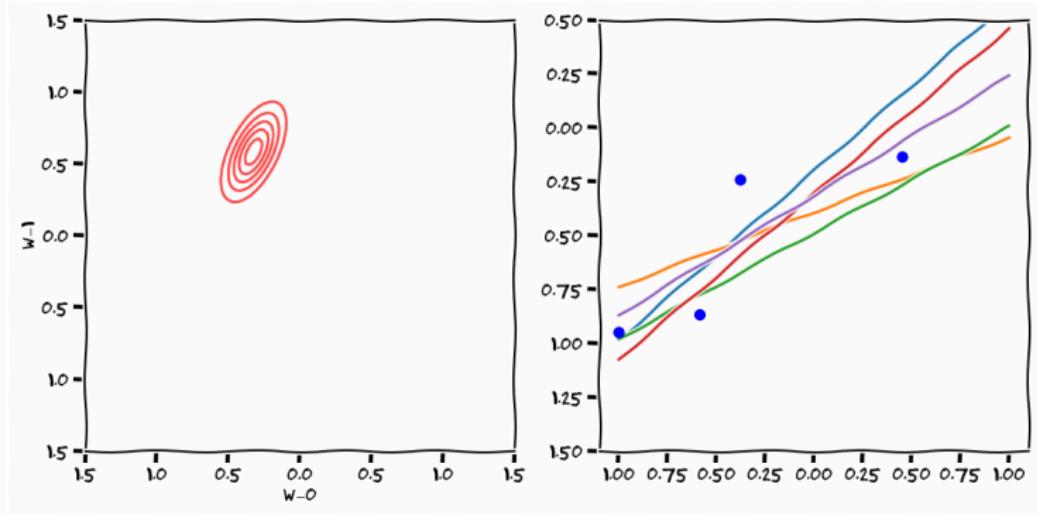
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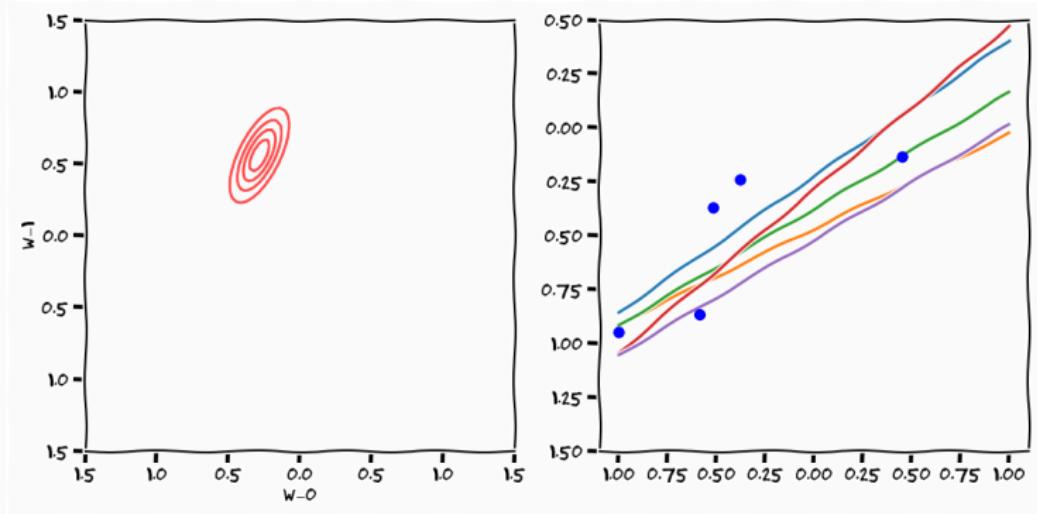
# Linear Regression Example



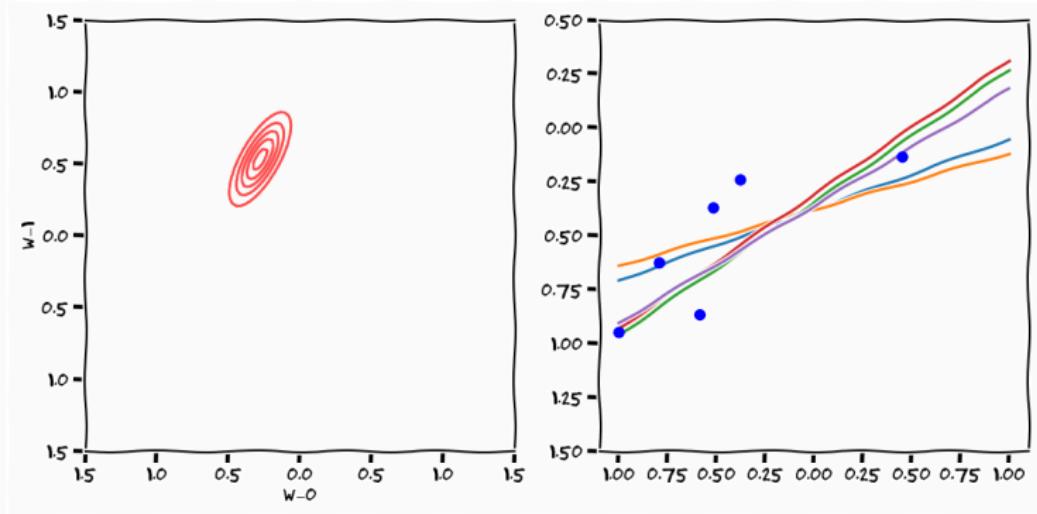
# Linear Regression Example



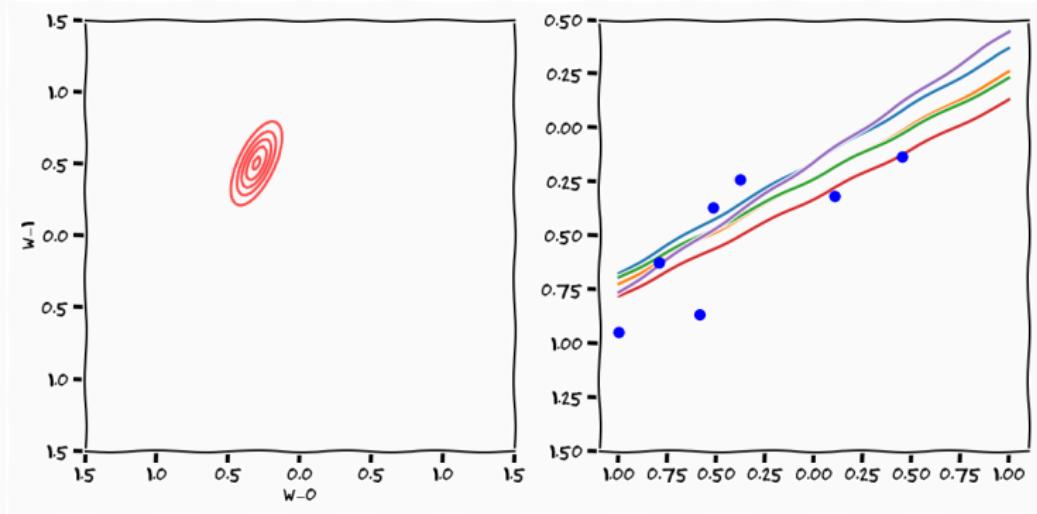
# Linear Regression Example



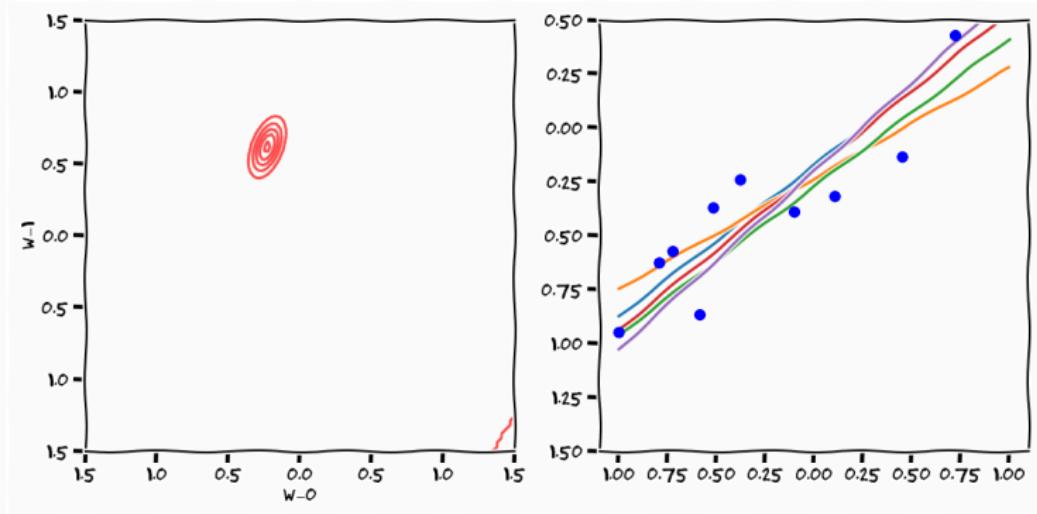
# Linear Regression Example



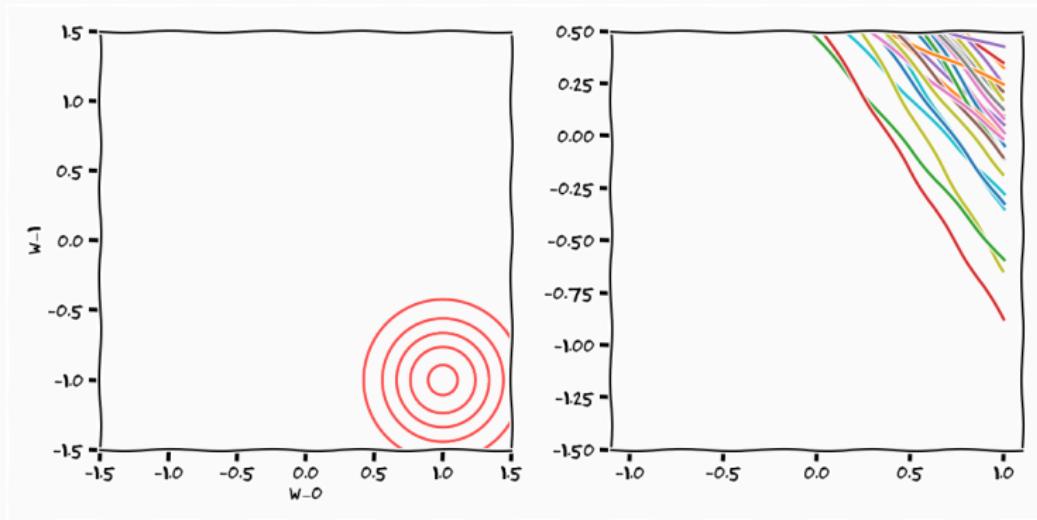
# Linear Regression Example



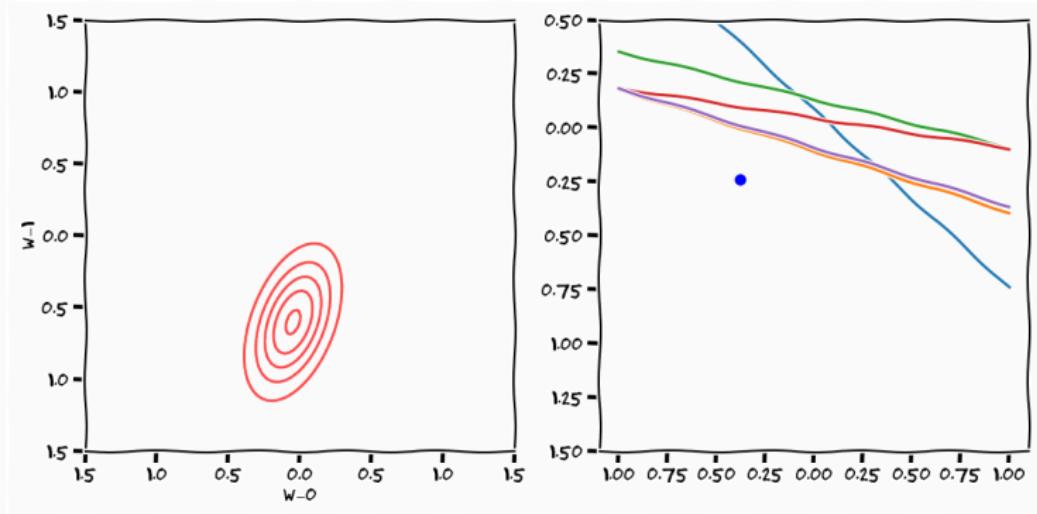
# Linear Regression Example



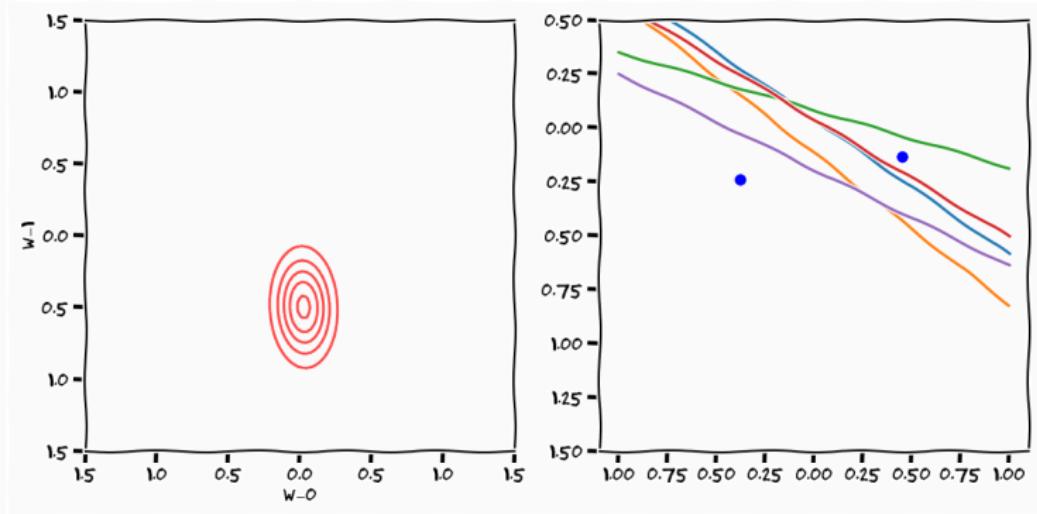
# Linear Regression Example



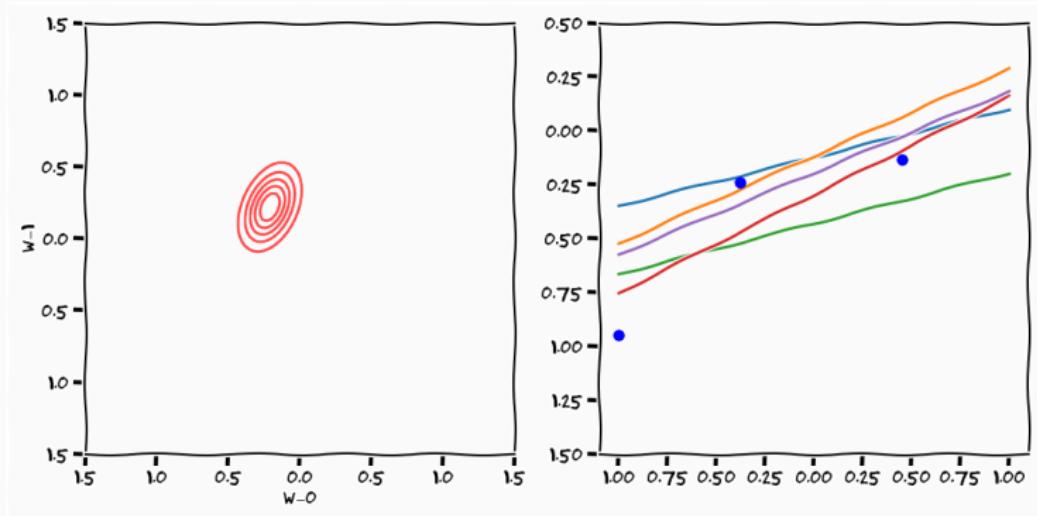
# Linear Regression Example



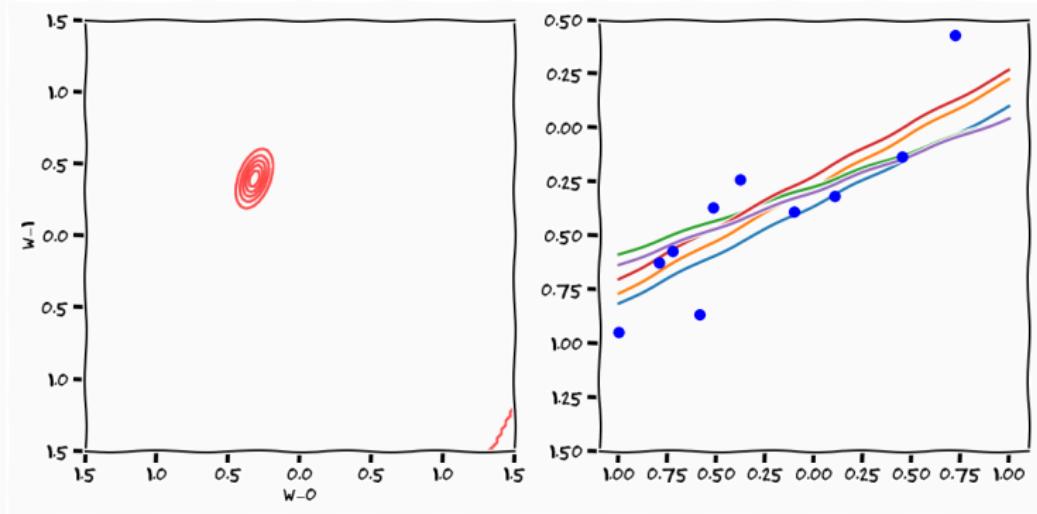
# Linear Regression Example



# Linear Regression Example



# Linear Regression Example



# Statistics or Machine Learning

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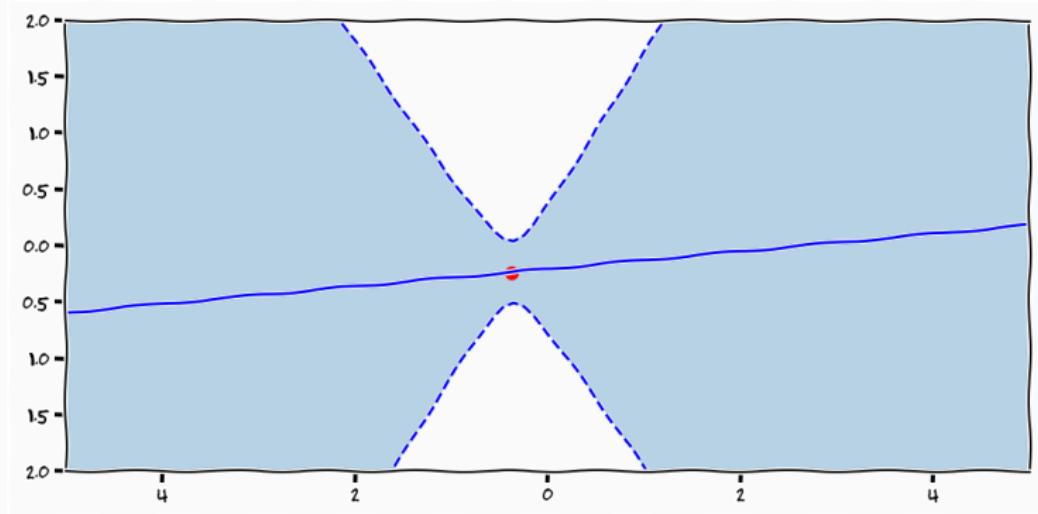
*"The difference between statistics and machine learning is that the former cares about parameters while the latter cares about prediction"*

*– Prof. Neil D. Lawrence*

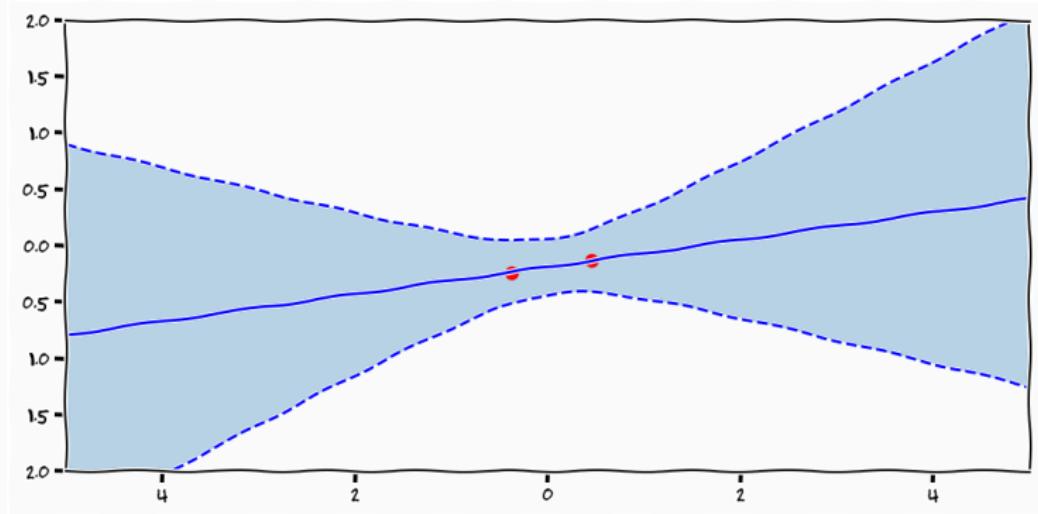
$$p(y_* | \mathbf{y}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) = \int p(y_* | \mathbf{x}_*, \mathbf{w}, \beta) p(\mathbf{w} | \mathbf{y}, \mathbf{X}, \alpha, \beta) d\mathbf{w}$$

- we do not really care about the value of  $w$  we care about new prediction  $y_*$  at location  $\mathbf{x}_*$
- look at the marginal distribution, i.e. when we average out the weight
- integrate a Gaussian over a Gaussian  $\Rightarrow$  Gaussian identities

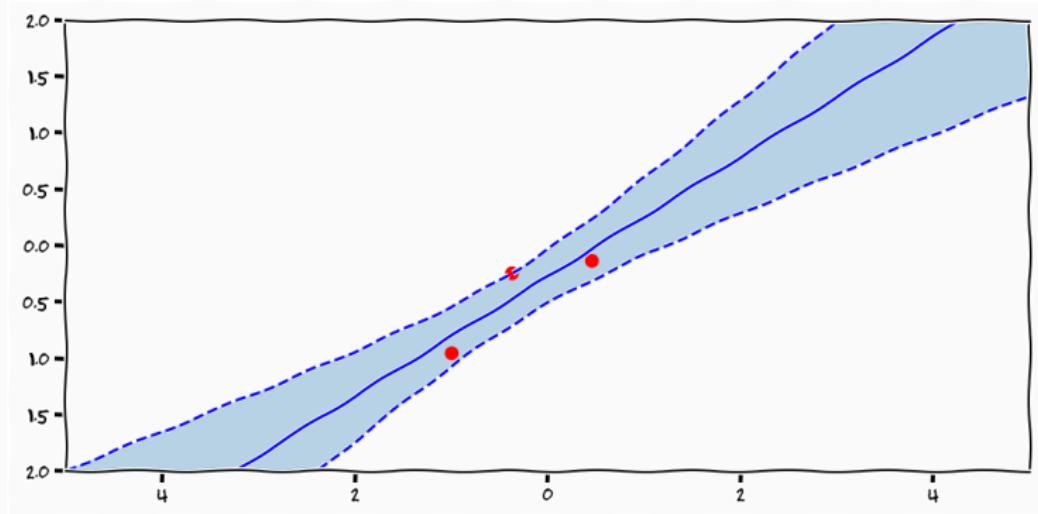
# Predictive Posterior



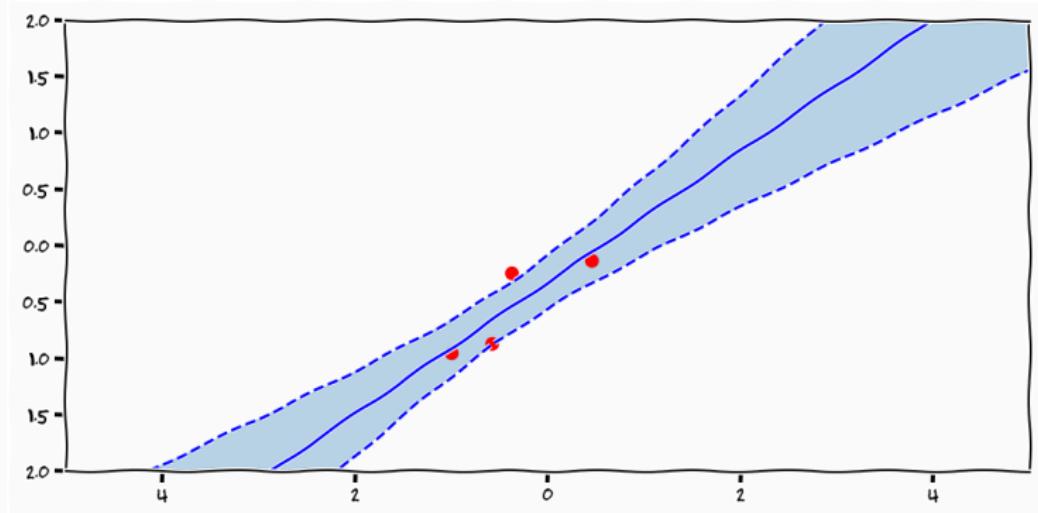
# Predictive Posterior



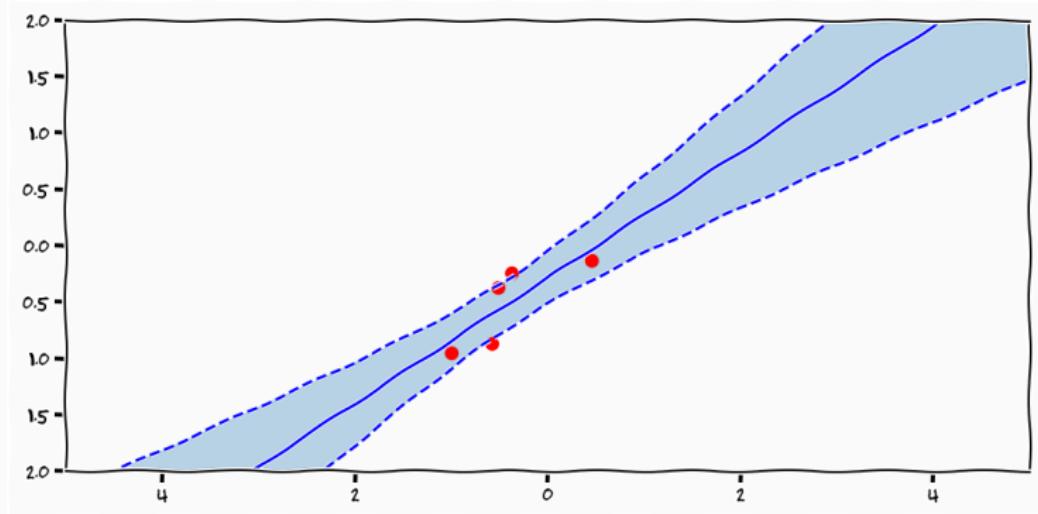
# Predictive Posterior



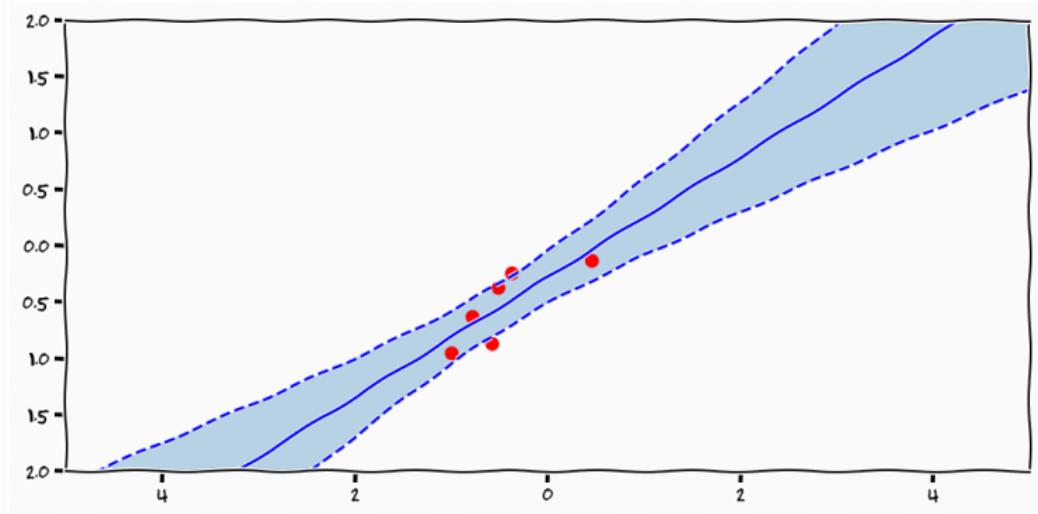
# Predictive Posterior



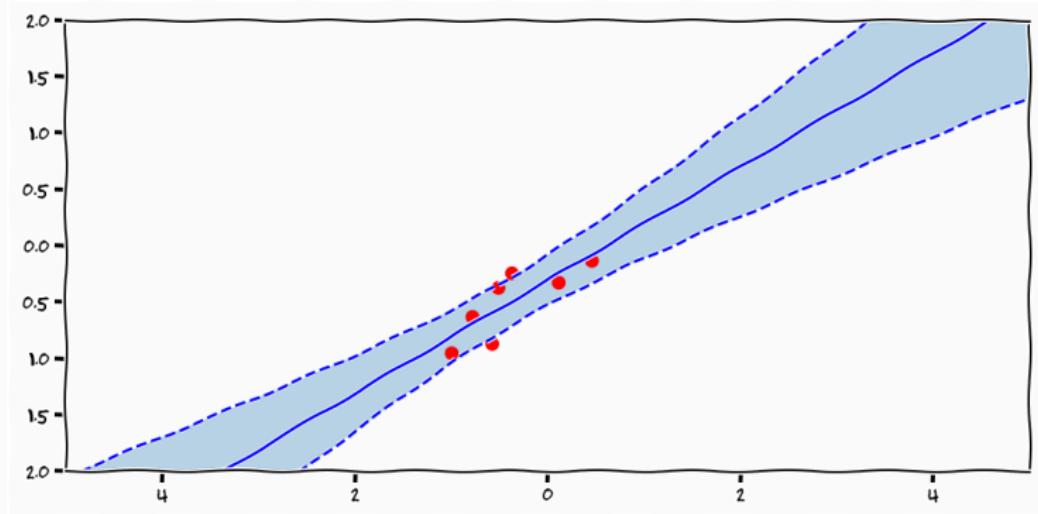
# Predictive Posterior



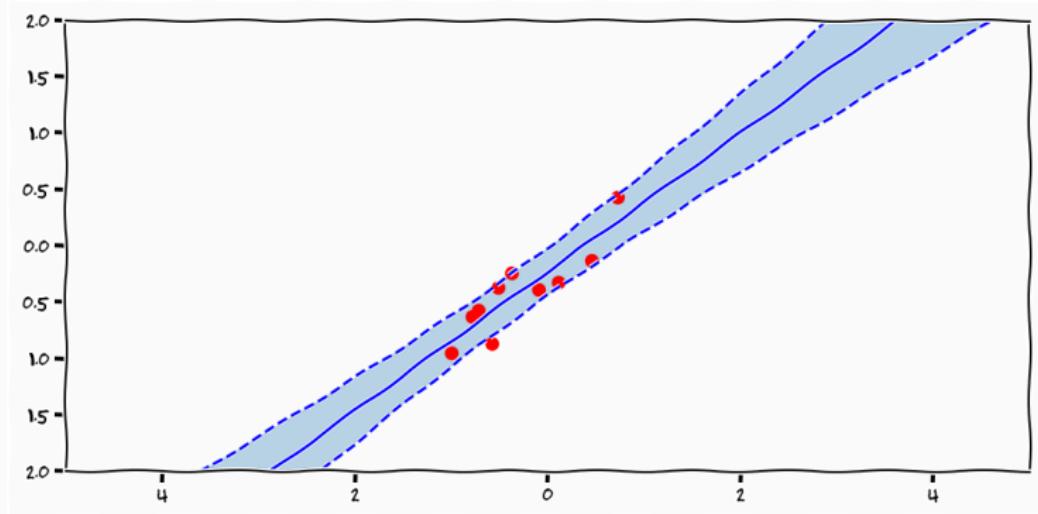
# Predictive Posterior



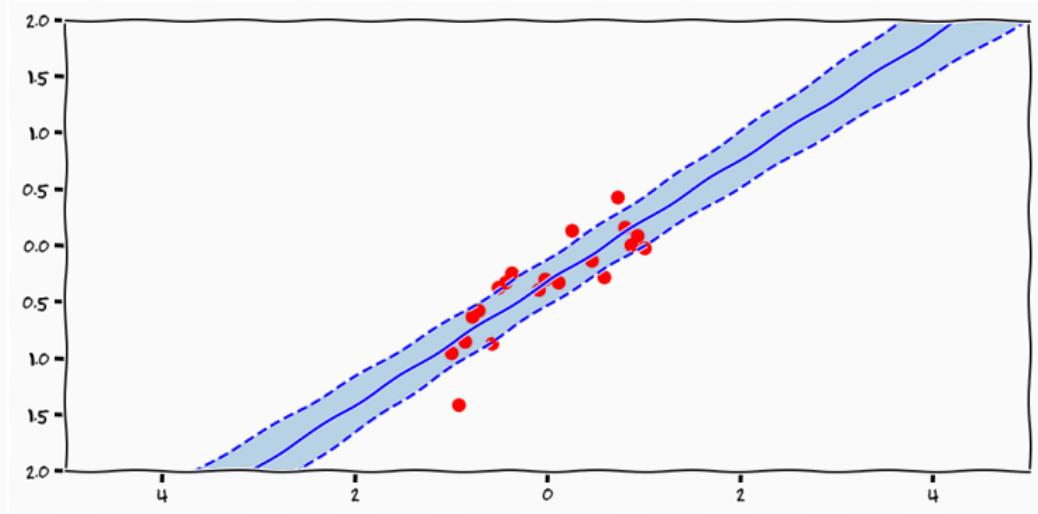
# Predictive Posterior



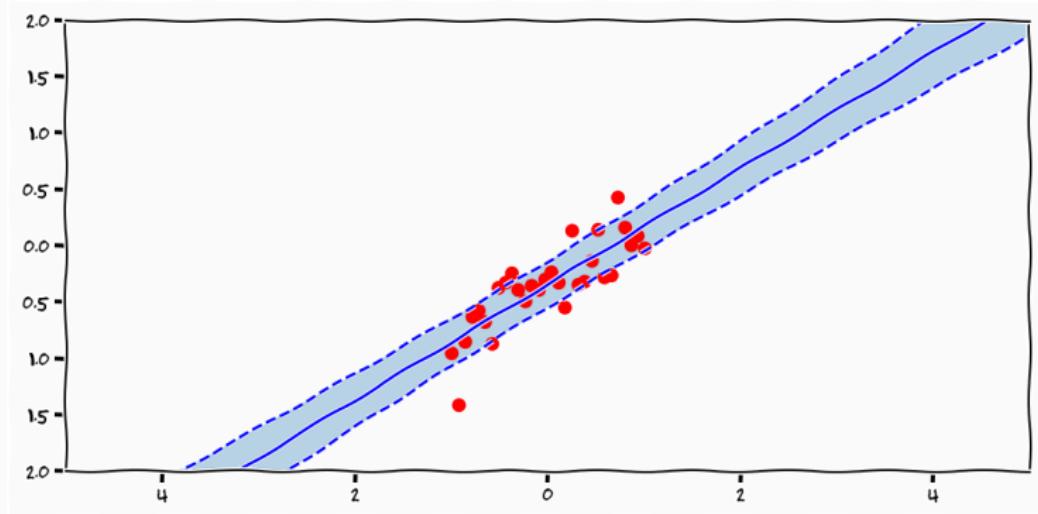
# Predictive Posterior



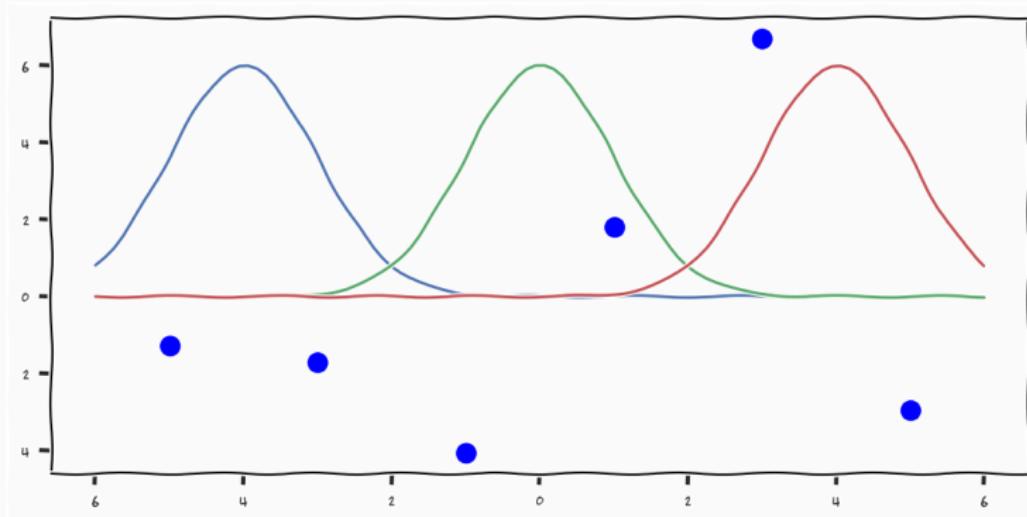
# Predictive Posterior



# Predictive Posterior



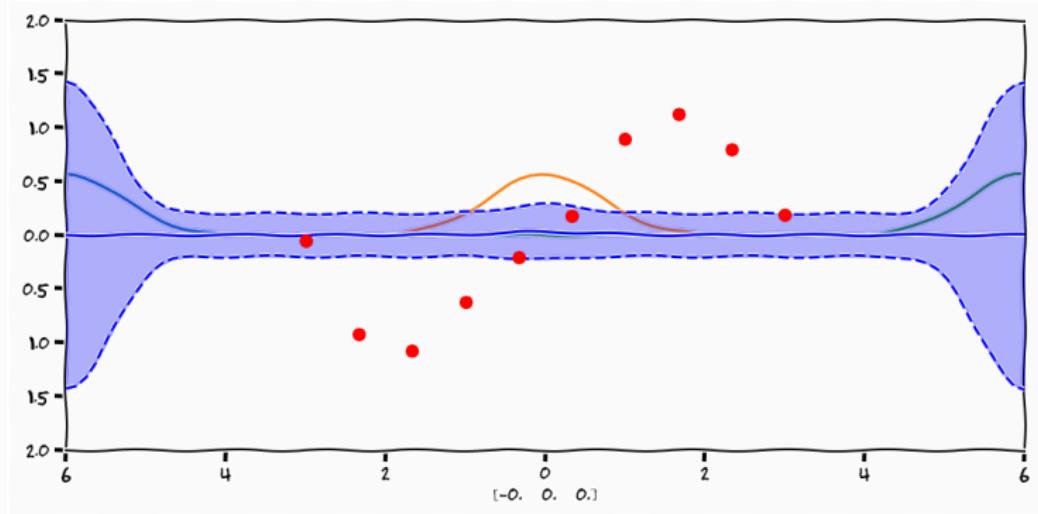
# Linear Regression



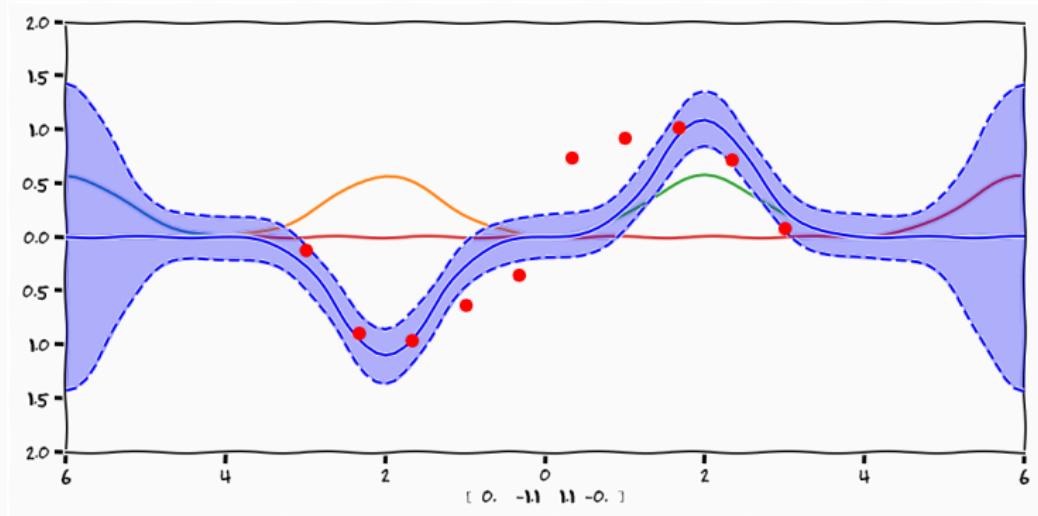
- Linear function only in parameters

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$$

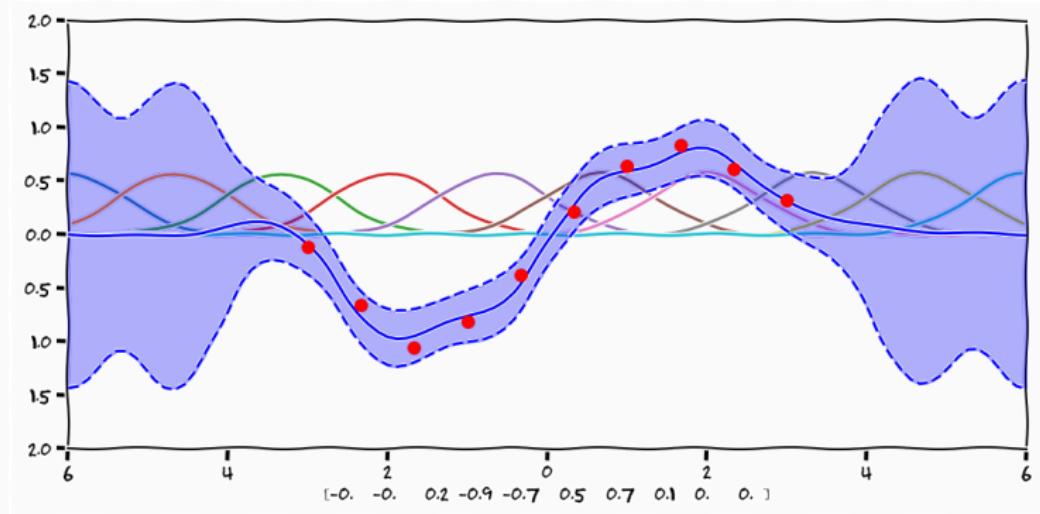
# Non-Linear Basis Functions



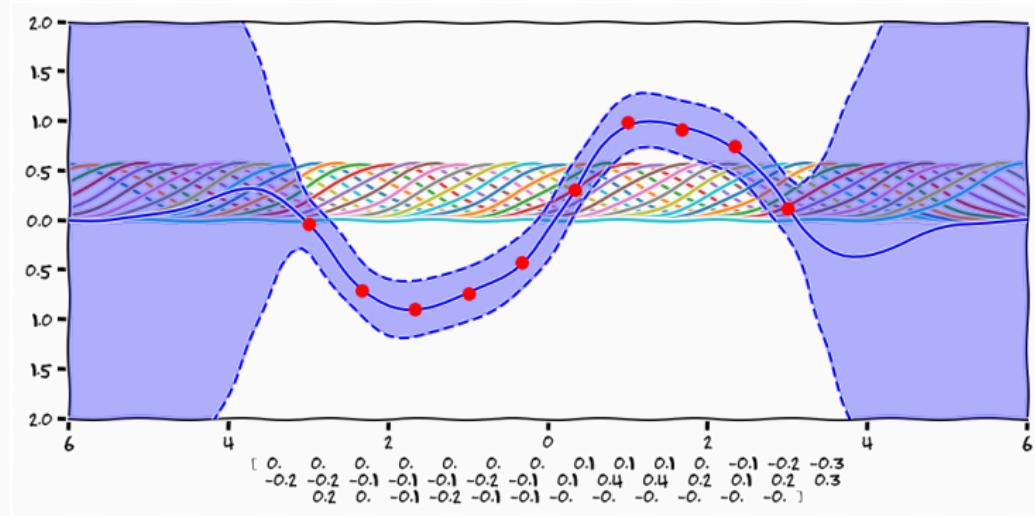
# Non-Linear Basis Functions



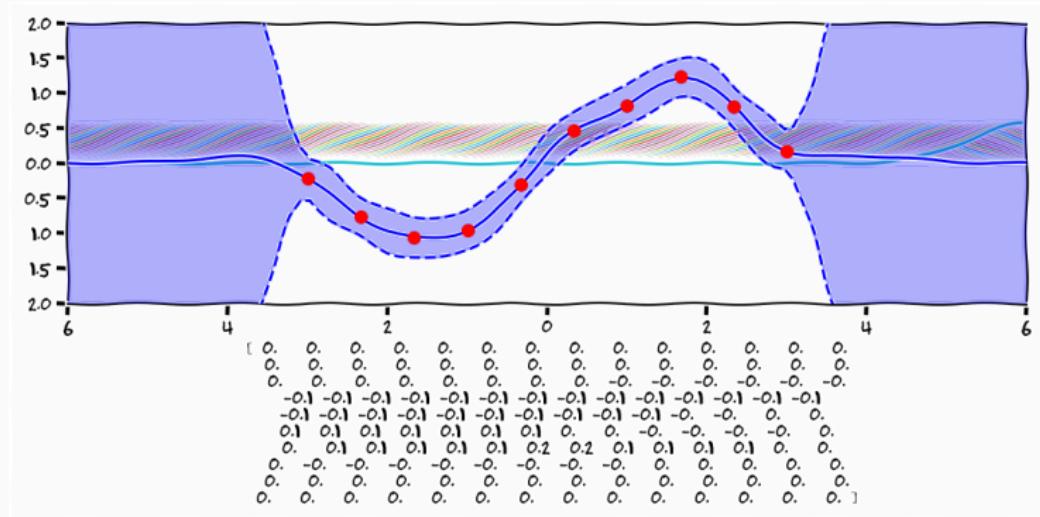
# Non-Linear Basis Functions



## Non-Linear Basis Functions



# Non-Linear Basis Functions



# Which Parametrisation

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- Should I use a line, polynomial, quadratic basis function?
- How many basis functions should I use?
- Likelihood won't help me
- How do we proceed?

# Regression Models

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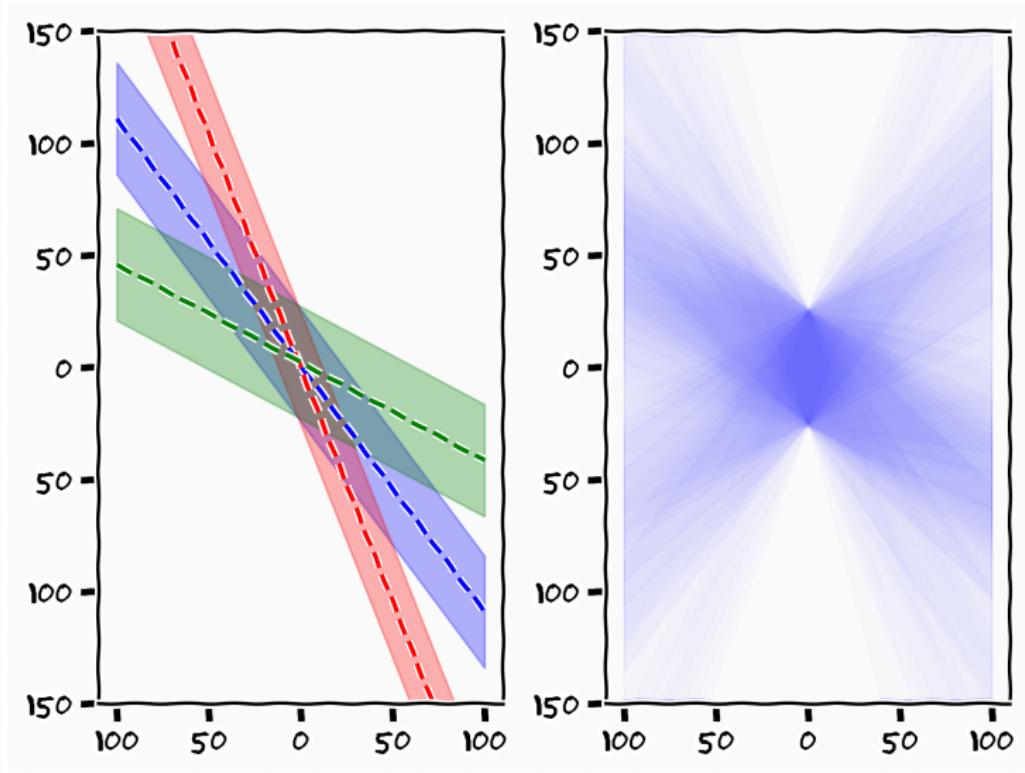
## Linear Model

$$p(y_i|x_i, \mathbf{w}) = \mathcal{N}(w_0 + w_1 \cdot x_i, \beta^{-1})$$

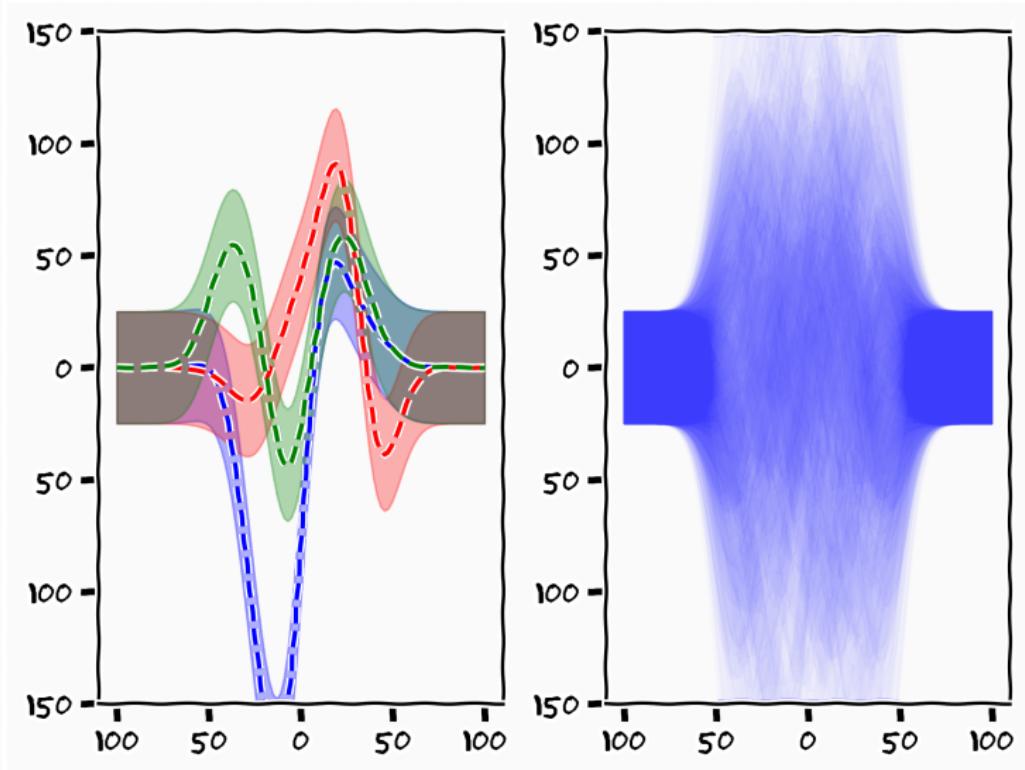
## Basis function

$$p(y_i|x_i, \mathbf{w}) = \mathcal{N}\left(\sum_{i=1}^6 w_i \phi(x_i), \beta^{-1}\right)$$

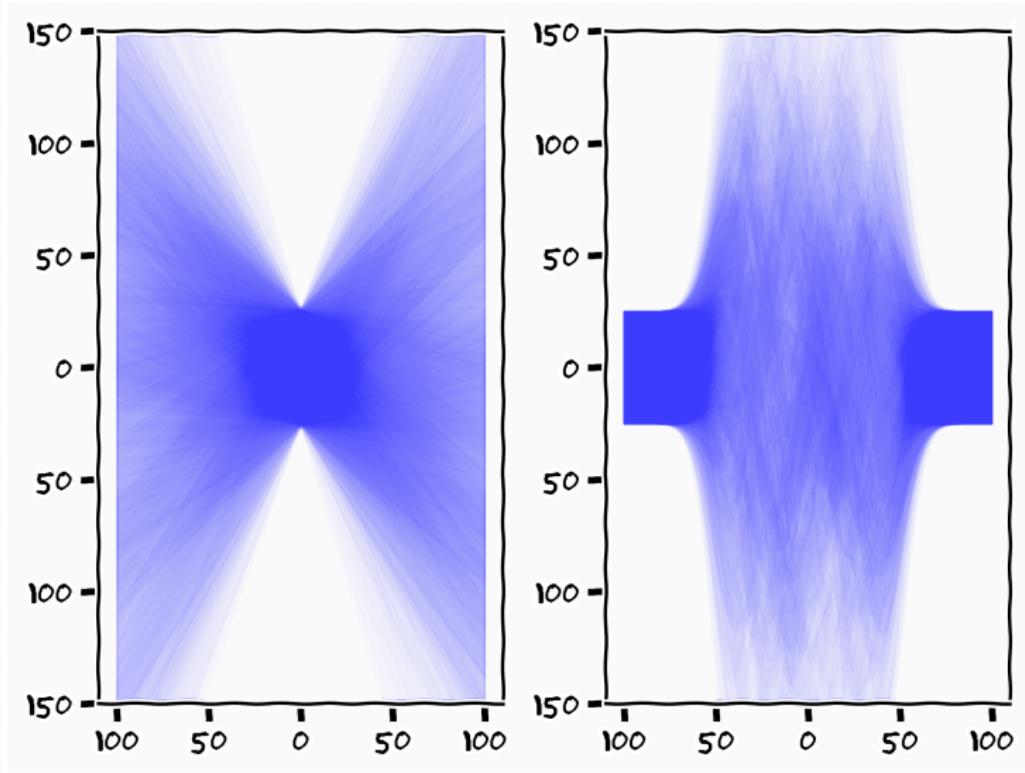
# Model 1



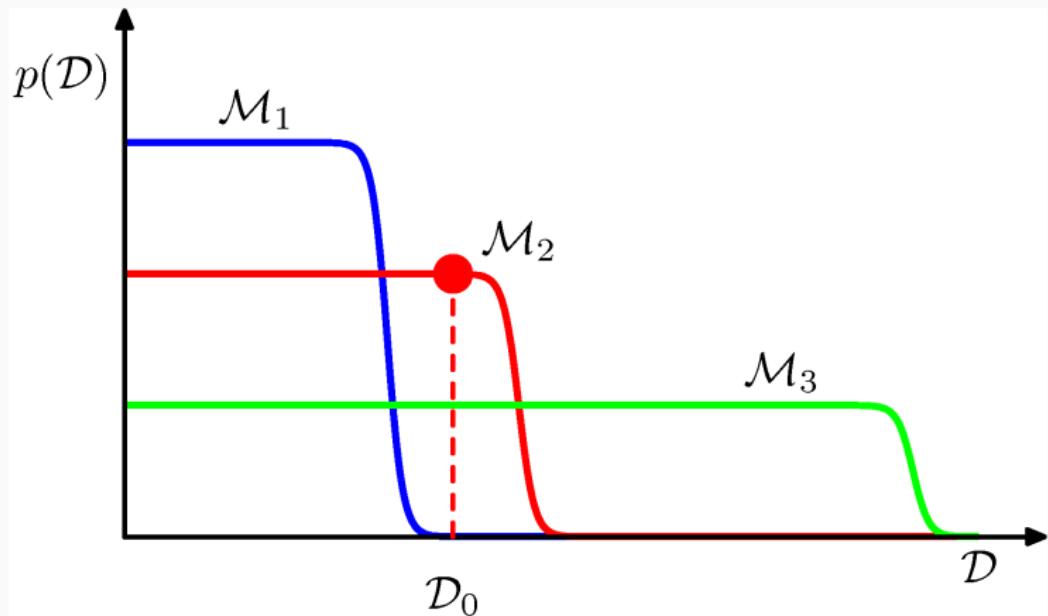
## Model 2



# Evidence



# Model Selection<sup>2</sup>



<sup>2</sup>David MacKay PhD Thesis

# Occams Razor

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## **Definition (Occams Razor)**

"All things being equal, the simplest solution tends to be the best one"

– William of Ockham

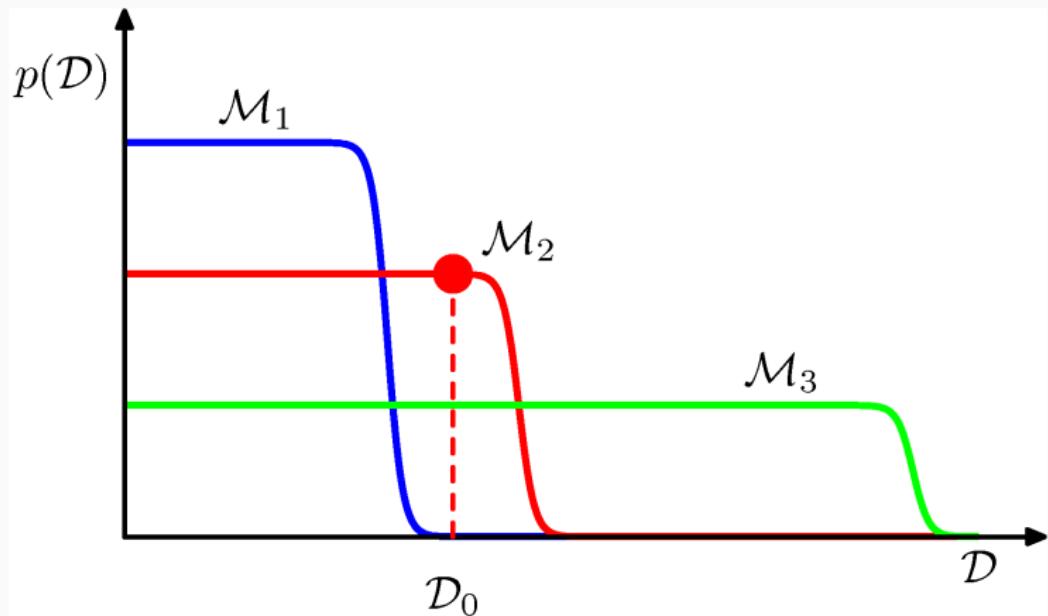
# What is Simple?<sup>3</sup>



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<sup>3</sup><https://www.imdb.com/title/tt8132700/>

# Model Selection<sup>2</sup>



<sup>2</sup>David MacKay PhD Thesis

## Summary

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## Summary

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- *That was a lot of philosophical nonsense to do something I did in school when I was 12*

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<sup>4</sup>we really hope so :-)

## Summary

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- *That was a lot of philosophical nonsense to do something I did in school when I was 12*
- The important thing was **not** "least squares" but how we reasoned to get to the result

---

<sup>4</sup>we really hope so :-)

## Summary

---

- *That was a lot of philosophical nonsense to do something I did in school when I was 12*
- The important thing was **not** "least squares" but how we reasoned to get to the result
- This reasoning will stay consistent through the course<sup>4</sup>

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<sup>4</sup>we really hope so :-)

# Practical

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- Bernoulli Trial

# Practical

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- Bernoulli Trial
- Linear regression

- Bernoulli Trial
- Linear regression
- Gaussian Identities

eof

## References

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## References

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-  Chomsky, Noam A and Jerry A Fodor (1980). "The inductivist fallacy". In: *Language and Learning: The Debate between Jean Piaget and Noam Chomsky*.
-  Laplace, Pierre Simon (1814). *A philosophical essay on probabilities*.

Does this make sense?

Posterior Variance

$$\mathbf{S}_N = (\mathbf{I}\alpha + \beta\mathbf{X}^T\mathbf{X})^{-1}$$

Posterior Mean

$$\mathbf{m}_N = \left( \frac{1}{\alpha}\mathbf{I} + \beta\mathbf{X}^T\mathbf{X} \right)^{-1} \beta\mathbf{X}^T\mathbf{y}$$

## Posterior Variance

$$\mathbf{S}_N = (\mathbf{I}\alpha + \beta\mathbf{X}^T\mathbf{X})^{-1}$$

$$= \left( \mathbf{I}\alpha + \beta \begin{bmatrix} \sum_i^N 1 & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{bmatrix} \right)^{-1} = \begin{bmatrix} \beta N + \alpha & \beta \sum_i x_i \\ \beta \sum_i x_i & \alpha + \beta \sum_i x_i^2 \end{bmatrix}^{-1}$$

$$= \frac{1}{(\beta N + \alpha)(\alpha + \beta \sum_i x_i^2) - (\beta \sum_i x_i)^2} \begin{bmatrix} \alpha + \beta \sum_i x_i^2 & -\beta \sum_i x_i \\ -\beta \sum_i x_i & \beta N + \alpha \end{bmatrix}$$

## Posterior Variance

$$\mathbf{S}_N = \frac{1}{(\beta N + \alpha)(\alpha + \beta \sum_i x_i^2) - (\beta \sum_i x_i)^2} \begin{bmatrix} \alpha + \beta \sum_i x_i^2 & -\beta \sum_i x_i \\ -\beta \sum_i x_i & \beta N + \alpha \end{bmatrix}$$

## Posterior Variance

$$\mathbf{S}_N = \frac{1}{(\beta N + \alpha)(\alpha + \beta \sum_i x_i^2) - (\beta \sum_i x_i)^2} \begin{bmatrix} \alpha + \beta \sum_i x_i^2 & -\beta \sum_i x_i \\ -\beta \sum_i x_i & \beta N + \alpha \end{bmatrix}$$

- Lets assume input is centered  $\Rightarrow \sum_i x_i = 0$

$$\begin{aligned}\mathbf{S}_N &= \frac{1}{(\beta N + \alpha)(\alpha + \beta \sum_i x_i^2)} \begin{bmatrix} \alpha + \beta \sum_i x_i^2 & 0 \\ 0 & \beta N + \alpha \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{\beta N + \alpha} & 0 \\ 0 & \frac{1}{\alpha + \beta \sum_i x_i^2} \end{bmatrix}\end{aligned}$$

## Posterior Mean

$$\begin{aligned}\mathbf{m}_N &= (\alpha \mathbf{I} + \beta \mathbf{X}^T \mathbf{X})^{-1} \beta \mathbf{X}^T \mathbf{y} \\ &= \beta \mathbf{S}_N \begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_N \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \\ &= \beta \mathbf{S}_N \begin{bmatrix} \sum_i y_i \\ \sum_i y_i x_i \end{bmatrix}\end{aligned}$$

## Posterior Mean

$$\mathbf{m}_N = \beta \mathbf{S}_N \begin{bmatrix} \sum_i y_i \\ \sum_i y_i x_i \end{bmatrix}$$

- Lets assume input is centered  $\Rightarrow \sum_i x_i = 0$

$$\begin{aligned}\mathbf{m}_N &= \beta \begin{bmatrix} \frac{1}{\beta N + \alpha} & 0 \\ 0 & \frac{1}{\alpha + \beta \sum_i x_i^2} \end{bmatrix} \begin{bmatrix} \sum_i y_i \\ \sum_i y_i x_i \end{bmatrix} \\ &= \begin{bmatrix} \frac{\beta \sum_i y_i}{\beta N + \alpha} \\ \frac{\beta \sum_i y_i x_i}{\alpha + \beta \sum_i x_i^2} \end{bmatrix}\end{aligned}$$

## Posterior Mean Slope

$$\tilde{w}_0 = \frac{\beta \sum_i y_i}{\beta N + \alpha}$$

$$p(w_0) = \mathcal{N}(w_0 | 0, \frac{1}{\alpha})$$

$$p(\epsilon) = \mathcal{N}(\epsilon | 0, \frac{1}{\beta})$$