

Machine Learning and the Physical World

Lecture 2 : Quantification of Beliefs

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Today

• Why understanding our ignorance is not just desirable but necessary for learning

Today

- Why understanding our ignorance is not just desirable but necessary for learning
- Why knowledge is subjective or relative

Today

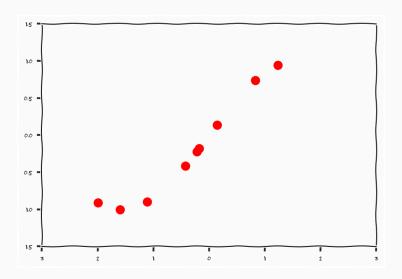
- Why understanding our ignorance is not just desirable but necessary for learning
- Why knowledge is subjective or relative
- Re-cap of linear regression

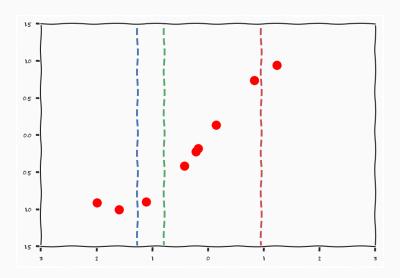
Inductive Reasoning

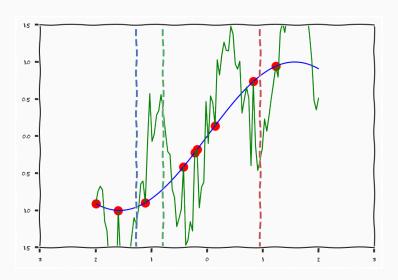
Inductive Reasoning

"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





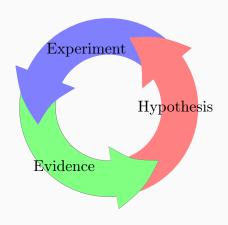


Inductive Reasoning II

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



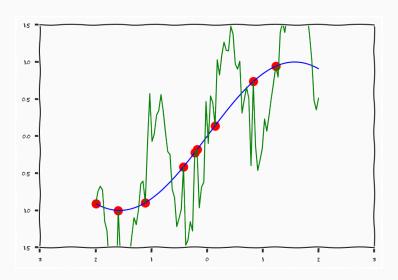
$$\mathsf{Data} + \mathsf{Model} \xrightarrow{Compute} \mathsf{Prediction}$$

"The Machine Learning Principle"1

"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

¹Chomsky et al., 1980



ullet space of functions

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

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

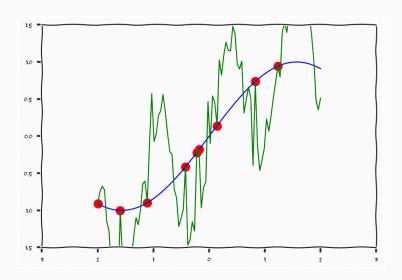
$$e(\mathcal{S}, \mathcal{A}, \mathcal{F}) = \mathbb{E}_{P(\{\mathcal{X}, \mathcal{Y}\})} [\ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y)]$$

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$$= \int \ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y) p(x, y) dx dy$$
$$\approx \frac{1}{M} \sum_{n=1}^{M} \ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x_n, y_n)$$

No Free Lunch

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 arbitary value



Assumptions: Algorithms







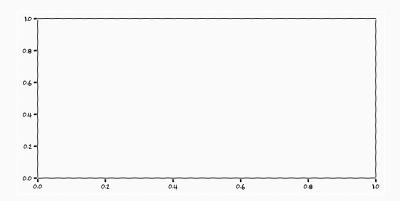
Statistical Learning

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

Assumptions: Biased Sample

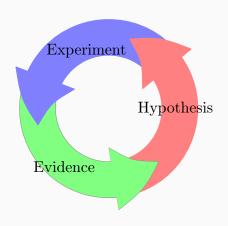
$$\mathcal{A}_{\mathcal{F}}(\boldsymbol{\mathcal{S}})$$

Assumptions: Hypothesis space

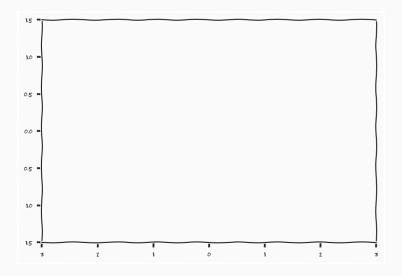


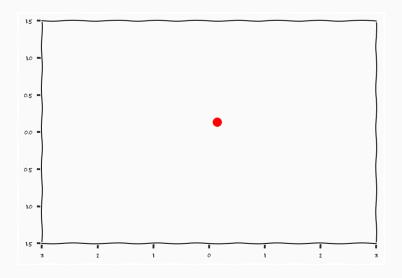
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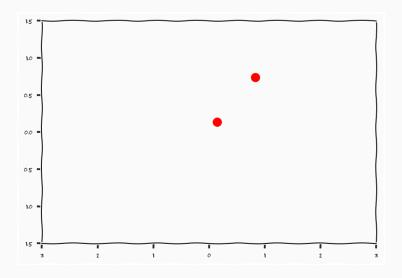
The Scientific Principle

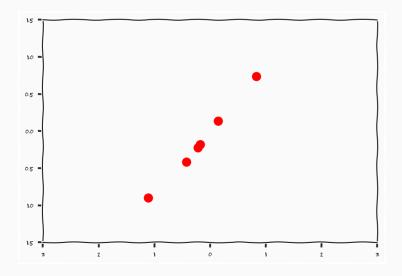


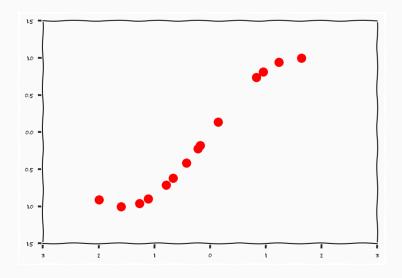
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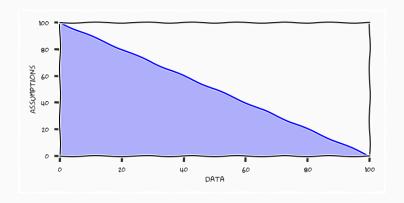




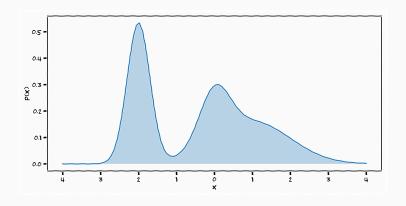




Data and Beliefs



Encoding Beliefs



Manipulation of Beliefs

Sum Rule

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

Product Rule

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

Baye's "Rule"

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

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

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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Semantics

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

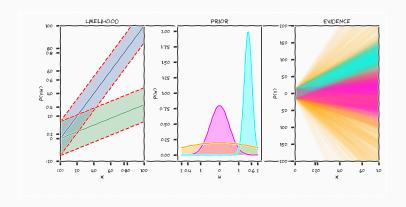
Likelihood How much evidence is there in the data for a specific hypothesis

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



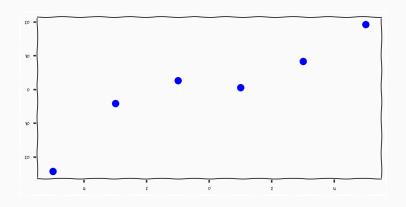
$$y = x \cdot w \pm 15$$

Uncertainty

Data Today

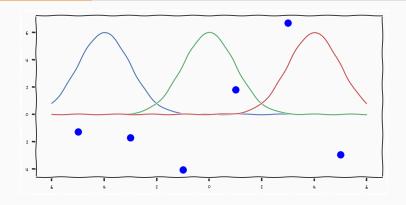
Model Friday

Computation Friday Week 4



Linear function in both parameters and data

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



• Linear function only in parameters

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

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

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

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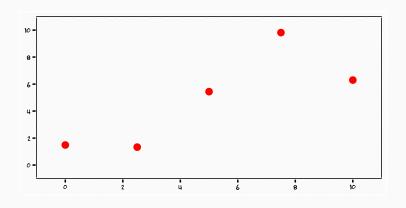
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 - formulate posterior (compute)
- Task 4 predict using my new belief (predict)
 - formulate predictive distribution

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

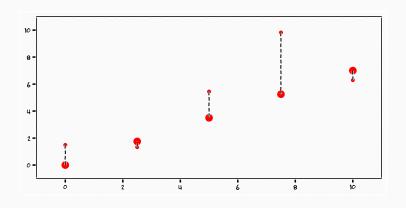
- We assume that we have been given data pairs $\{y_i, \mathbf{x}_i\}_{i=1}^N$ corrupted by addative noise
- We assume that the distribution of the noise follows a Gaussian

Explaining Away



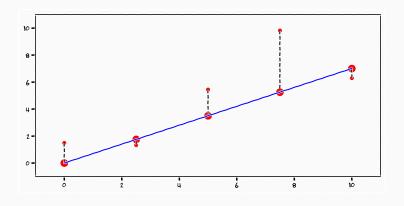
$$y = \mathbf{w}^{\mathrm{T}} x + \epsilon$$

Explaining Away



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

Explaining Away



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

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

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

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

Likelihood

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

Independence

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

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

• Likelihood is Gaussian in w

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

• Likelihood is Gaussian in w

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

• Conjugate Prior

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

• Likelihood is Gaussian in w

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

• Conjugate Prior

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

Posterior

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

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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

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Posterior

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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 is Gaussian

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

Identification

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \frac{p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})}{\int p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})dw} \propto p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

• Posterior is Gaussian

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

Identification

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \frac{p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})}{\int p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})dw} \propto p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

Posterior

$$\mathbf{m}_{N} = \left(\mathbf{S}_{0}^{-1} + \beta \mathbf{X}^{\mathrm{T}} \mathbf{X}\right)^{-1} \left(S_{0}^{-1} \mathbf{m}_{0} + \beta \mathbf{X}^{\mathrm{T}} \mathbf{y}\right)$$
$$\mathbf{S}_{N} = \left(\mathbf{S}_{0}^{-1} + \beta \mathbf{X}^{\mathrm{T}} \mathbf{X}\right)^{-1}$$

• Assumption Zero mean isotropic Gaussian

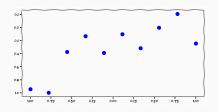
$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|0, \alpha^{-1}\mathbf{I})$$

• Assumption Zero mean isotropic Gaussian

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

Posterior

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



Model

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

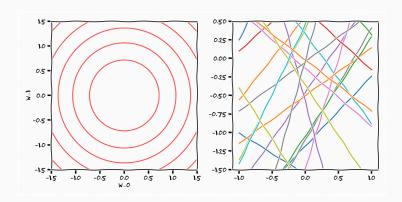
Data

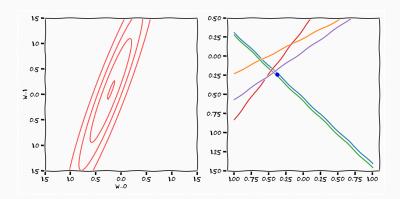
$$f(x, \mathbf{a}) = a_0 + a_1 x, \ \{a_0, a_1\} = \{-0.3, 0.5\}$$

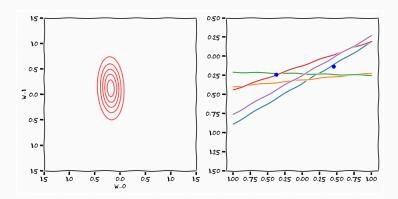
 $y = f(x, \mathbf{a}) + \epsilon, \ \epsilon \sim \mathcal{N}(0, 0.2^2)$

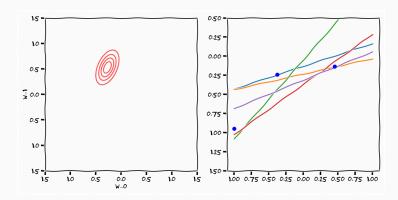
Prior

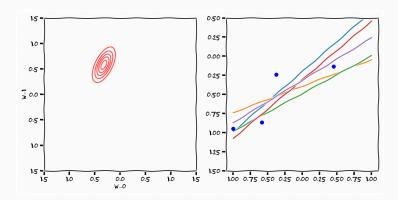
$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, 2.0 \cdot \mathbf{I})$$

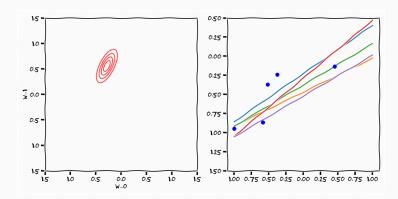


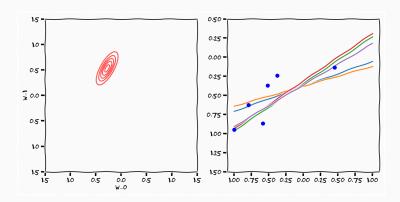


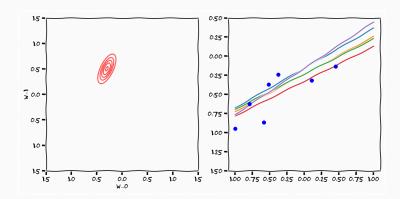


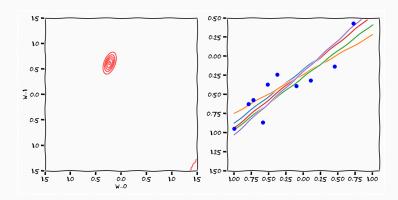


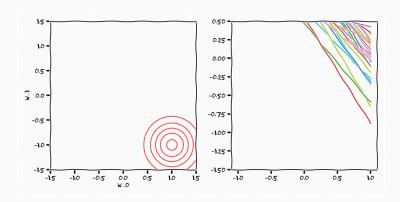


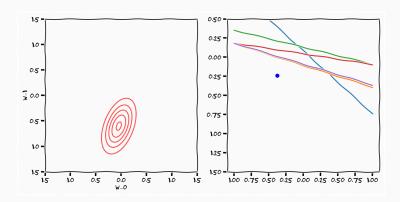


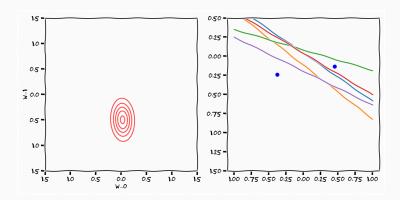


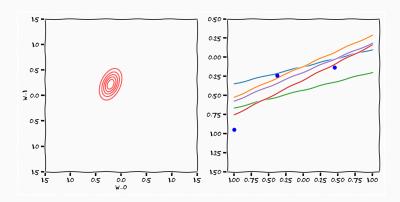


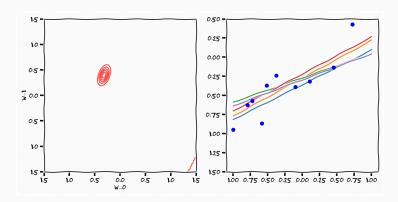




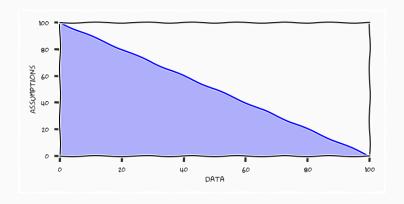




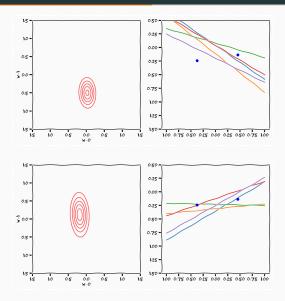




Data and Beliefs



Knowledge is Relative



Statistics or Machine Learning

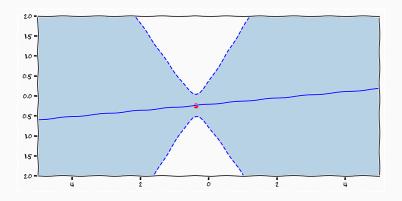
"The difference between statistics and machine learning is that the former cares about parameters while the latter cares about prediction"

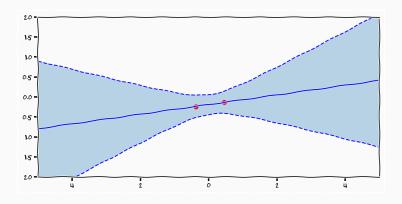
- Prof. Neil D. Lawrence

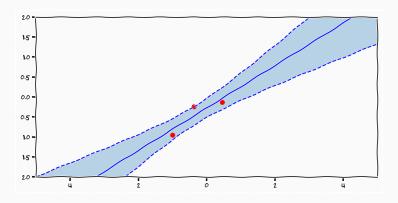
Prediction

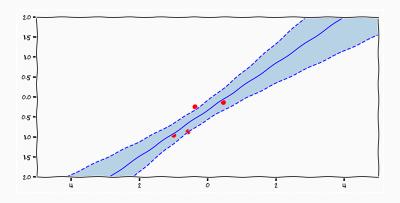
$$p(y_*|\mathbf{y}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) = \int p(y_*|\mathbf{x}_*, \mathbf{w}, \beta) p(\mathbf{w}|\mathbf{y}, \mathbf{X}, \alpha, \beta) d\mathbf{w}$$

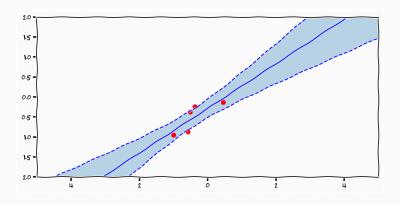
- we do not really care about the value of w we care about new prediction y_* at location \mathbf{x}_*
- look at the marginal distribution, i.e. when we average out the weight
- ullet integrate a Gaussian over a Gaussian \Rightarrow Gaussian identities

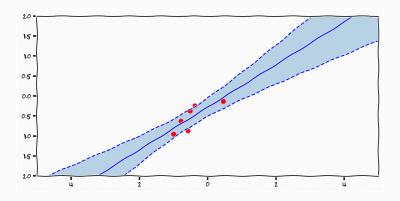


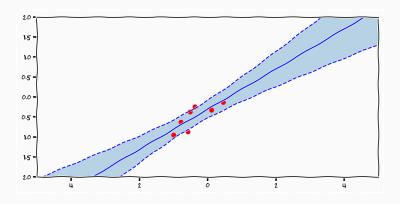


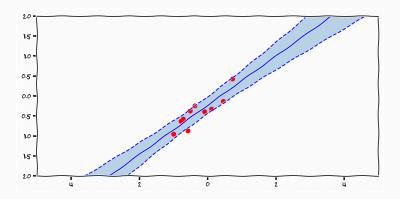


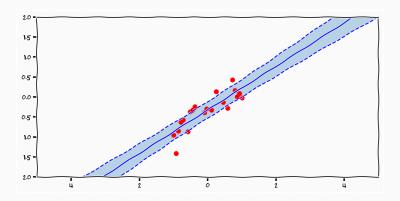


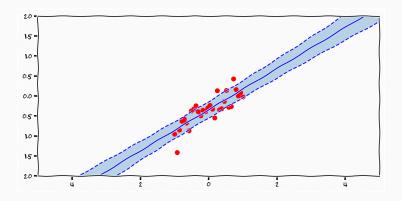




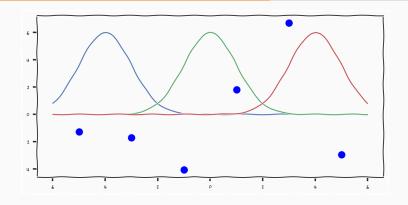








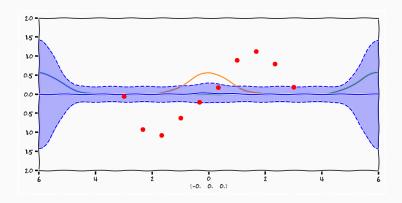
Linear Regression

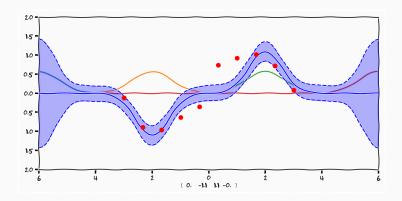


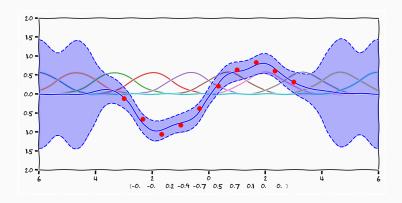
• Linear function only in parameters

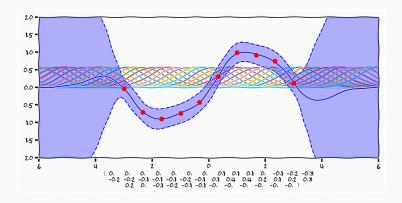
$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

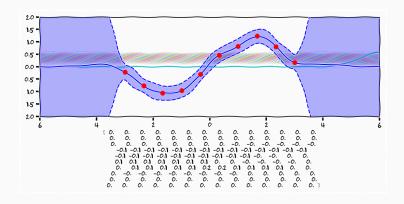
Non-Linear Basis Functions











• That was a lot of philosphical nonsense to do something I did in school when I was 12

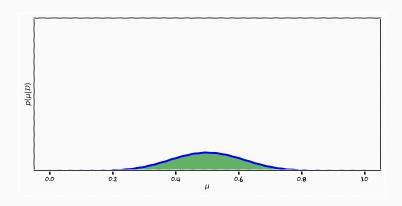
 $^{^{2}}$ we really hope so :-)

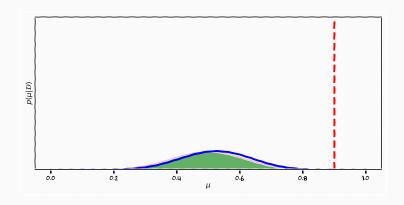
- That was a lot of philosphical nonsense to do something I did in school when I was 12
- The important thing was not "least squares" but how we reasoned to get to the result

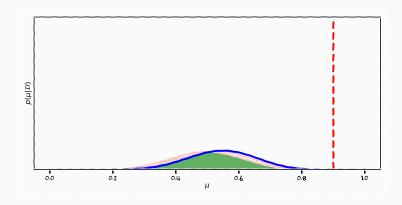
²we really hope so :-)

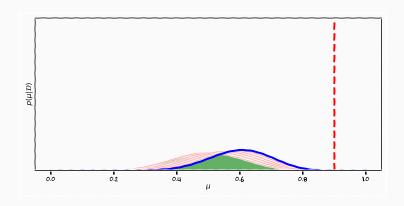
- That was a lot of philosphical nonsense to do something I did in school when I was 12
- The important thing was not "least squares" but how we reasoned to get to the result
- This reasoning will stay consistent through the course²

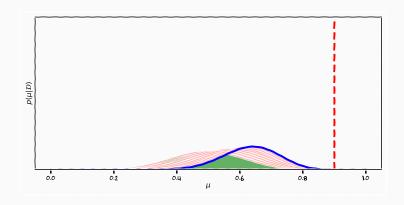
²we really hope so :-)

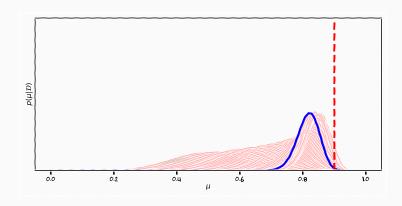


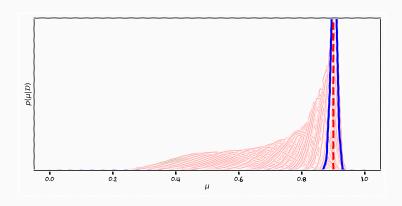


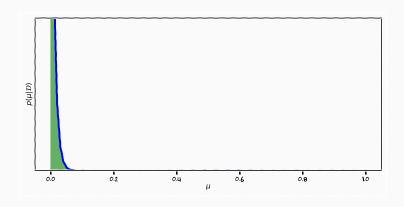


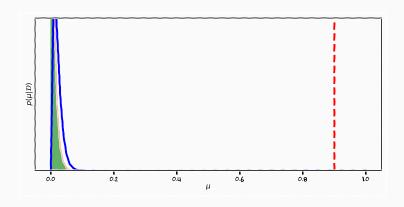


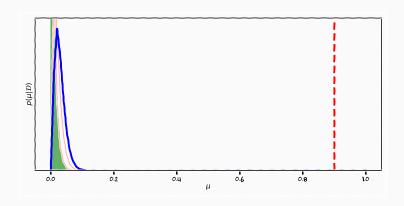


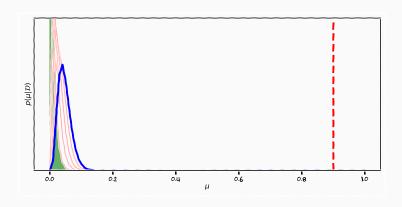


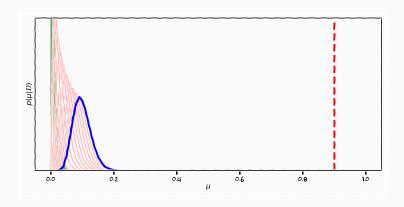


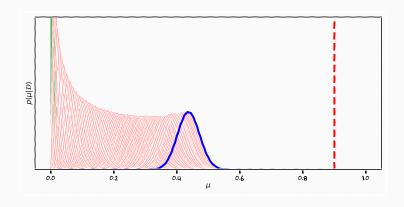


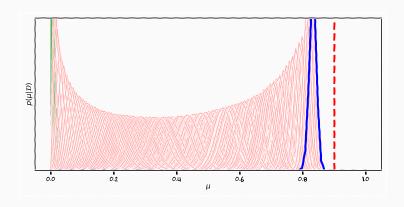


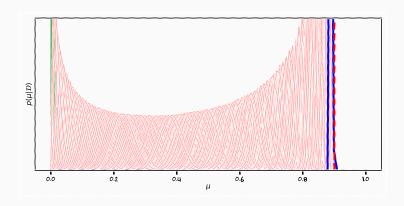




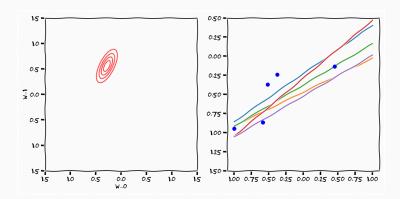








Linear Regression



Gaussian Identities

$$p(x_1, x_2)$$
 $p(x1)$ $p(x1 \mid x_2)$

eof

References

References

- 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

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

Posterior Mean

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

Posterior Variance

$$\mathbf{S}_{N} = \left(\mathbf{I}\alpha + \beta \mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1}$$

$$= \left(\mathbf{I}\alpha + \beta \begin{bmatrix} \sum_{i=1}^{N} 1 & \sum_{i=1}^{N} x_{i} \\ \sum_{i=1}^{N} x_{i} & \sum_{i=1}^{N} x_{i} \end{bmatrix} \right)^{-1} = \begin{bmatrix} \beta N + \alpha & \beta \sum_{i=1}^{N} x_{i} \\ \beta \sum_{i=1}^{N} x_{i} & \alpha + \beta \sum_{i=1}^{N} x_{i} \end{bmatrix}^{-1}$$

$$\left\{ \sum_{i} x_{i} \sum_{i} x_{i}^{2} \right\}$$

$$= \frac{1}{(\beta N + \alpha)(\alpha + \beta \sum_{i} x_{i}^{2}) - (\beta \sum_{i} x_{i})^{2}} \left[\begin{array}{cc} \alpha + \beta \sum_{i} x_{i}^{2} & -\beta \sum_{i} x_{i} \\ -\beta \sum_{i} x_{i} & \beta N + \alpha \end{array} \right]$$

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 $\Rightarrow \sum_i x_i = 0$

$$\mathbf{S}_{N} = \frac{1}{(\beta N + \alpha)(\alpha + \beta \sum_{i} x_{i}^{2})} \begin{bmatrix} \alpha + \beta \sum_{i} x_{i}^{2} & 0 \\ 0 & \beta N + \alpha \end{bmatrix}$$
$$= \begin{bmatrix} \frac{1}{\beta N + \alpha} & 0 \\ 0 & \frac{1}{\alpha + \beta \sum_{i} x_{i}^{2}} \end{bmatrix}$$

Posterior Mean

$$\mathbf{m}_{N} = (\alpha \mathbf{I} + \beta \mathbf{X}^{\mathrm{T}} \mathbf{X})^{-1} \beta \mathbf{X}^{\mathrm{T}} \mathbf{y}$$

$$= \beta \mathbf{S}_{N} \begin{bmatrix} 1 & \dots & 1 \\ x_{1} & \dots & x_{N} \end{bmatrix} \begin{bmatrix} y_{1} \\ \vdots \\ y_{N} \end{bmatrix}$$

$$= \beta \mathbf{S}_{N} \begin{bmatrix} \sum_{i} y_{i} \\ \sum_{i} y_{i} x_{i} \end{bmatrix}$$

Posterior Mean

$$\mathbf{m}_N = \beta \mathbf{S}_N \left[\begin{array}{c} \sum_i y_i \\ \sum_i y_i x_i \end{array} \right]$$

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

$$\mathbf{m}_{N} = \beta \begin{bmatrix} \frac{1}{\beta N + \alpha} & 0 \\ 0 & \frac{1}{\alpha + \beta \sum_{i} x_{i}^{2}} \end{bmatrix} \begin{bmatrix} \sum_{i} y_{i} \\ \sum_{i} y_{i} x_{i} \end{bmatrix}$$
$$= \begin{bmatrix} \frac{\beta \sum_{i} y_{i}}{\beta N + \alpha} \\ \frac{\beta \sum_{i} y_{i} x_{i}}{\alpha + \beta \sum_{i} x_{i}^{2}} \end{bmatrix}$$

Posterior Mean Slope

$$\tilde{w}_0 = \frac{\beta \sum_i y_i}{\beta N + \alpha}$$
$$p(w_0) = \mathcal{N}(w_0|0, \frac{1}{\alpha})$$
$$p(\epsilon) = \mathcal{N}(\epsilon|0, \frac{1}{\beta})$$

Which Parametrisation

- 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

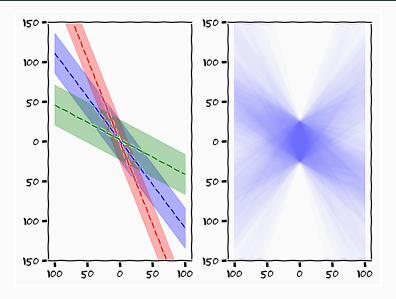
Linear Linear Model

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

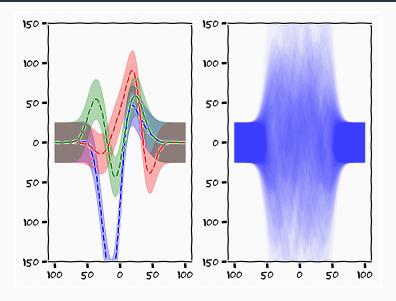
Basis function

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

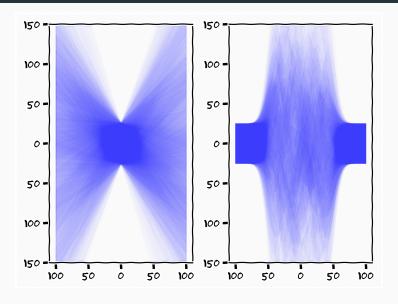
Model 1



Model 2

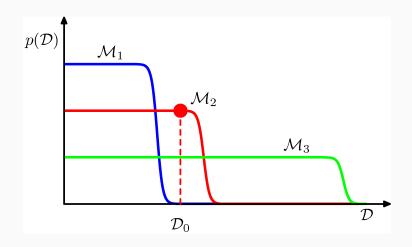


Evidence



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Model Selection³



³David MacKay PhD Thesis

Occams Razor



Occams Razor

Definition (Occams Razor)
"All things being equal, the simplest solution tends to be the best one"

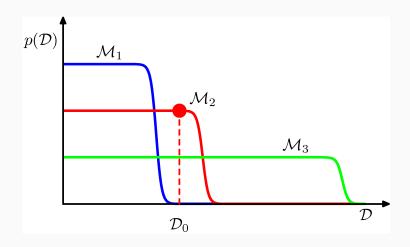
- William of Ockham

What is Simple?⁴



⁴https://www.imdb.com/title/tt8132700/

Model Selection³



³David MacKay PhD Thesis