Lecture 6

Bayesian Regression & Introduction to Deep Learning

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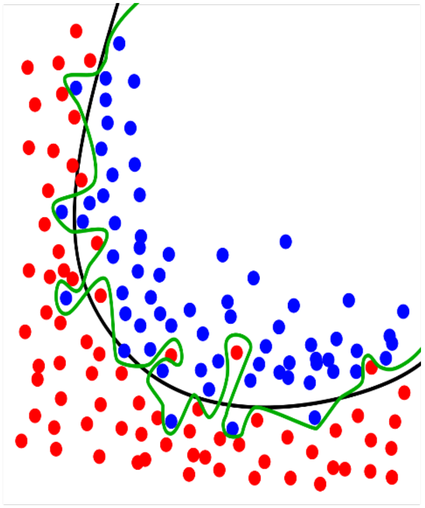
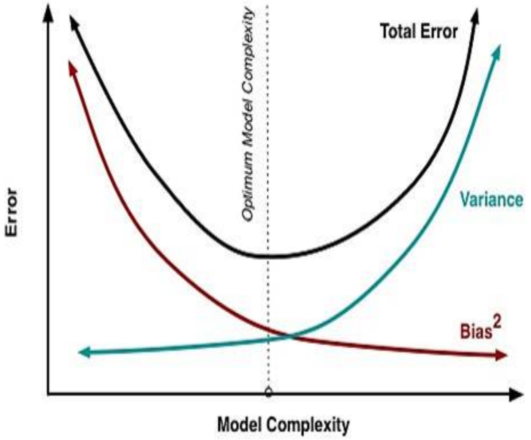
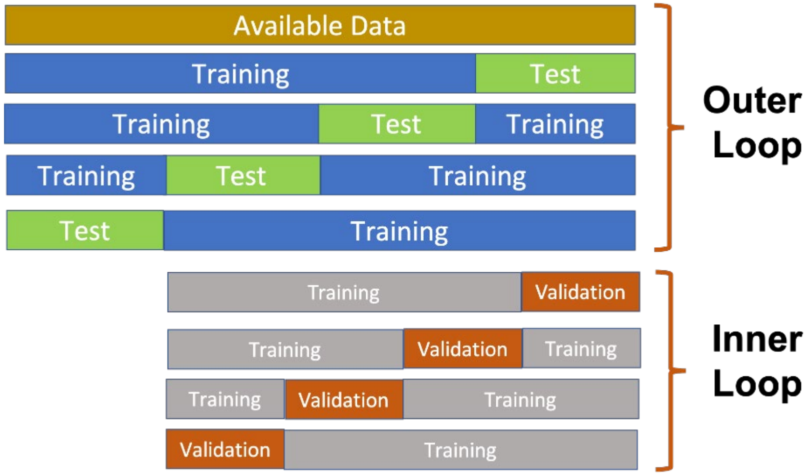
COM4509/6509: Machine Learning & Adaptive Intelligence

Review of previous lecture(s)

- Linear regression: $y = mx + c$; $y = \mathbf{w}^{T}\mathbf{x} + b$; $\mathbf{y} = \mathbf{W}\mathbf{x} + \mathbf{b}$
- Overfitting, bias-variance trade-off, cross validation







Available Data

Training | Test

Training | Test | Training

Training | Test | Training

Test | Training

Outer Loop

Training | Validation

Training | Validation | Training

Training | Validation | Training

Validation | Training

Inner Loop

Question

Our data is partitioned into three sets: training set, validation set, and test set. We train and tune our ML model on the validation set, getting an error E_{val}. We test this model on the test set, getting an error of E_{tst}.

Which case is the mostly likely to be ***overfitting****?*

A. $E_{val} << E_{tst}$

B. $E_{val} >> E_{tst}$

C. $E_{val} = E_{tst}$

Week 6 Contents / Objectives

Part A

- Bayesian Inference
- Bayesian Linear Regression
- Predictive Distribution

Part B

- Computational Graph
- PyTorch: A Deep Learning Library

Week 6 Contents / Objectives

Part A

- **Bayesian Inference**
- Bayesian Linear Regression
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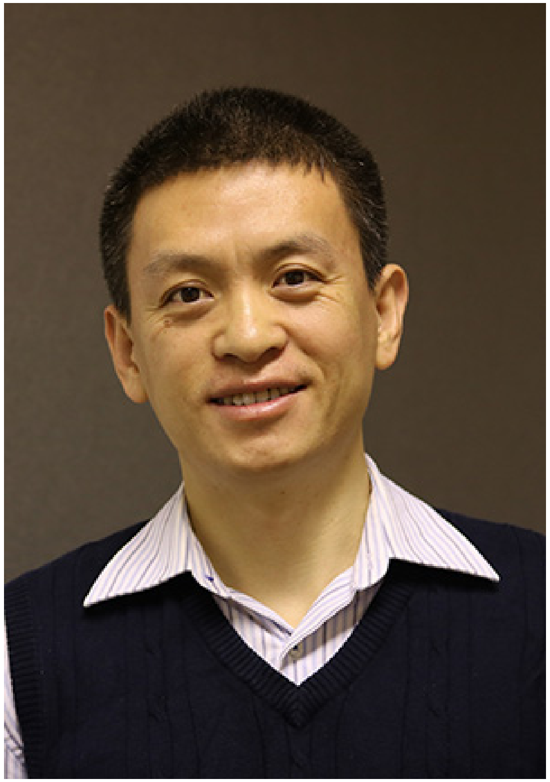
Question

- Which year was this photo taken?
  A. 1996
  B. 2006
  C. 2016
  D. 2026



Bayesian statistics

new data

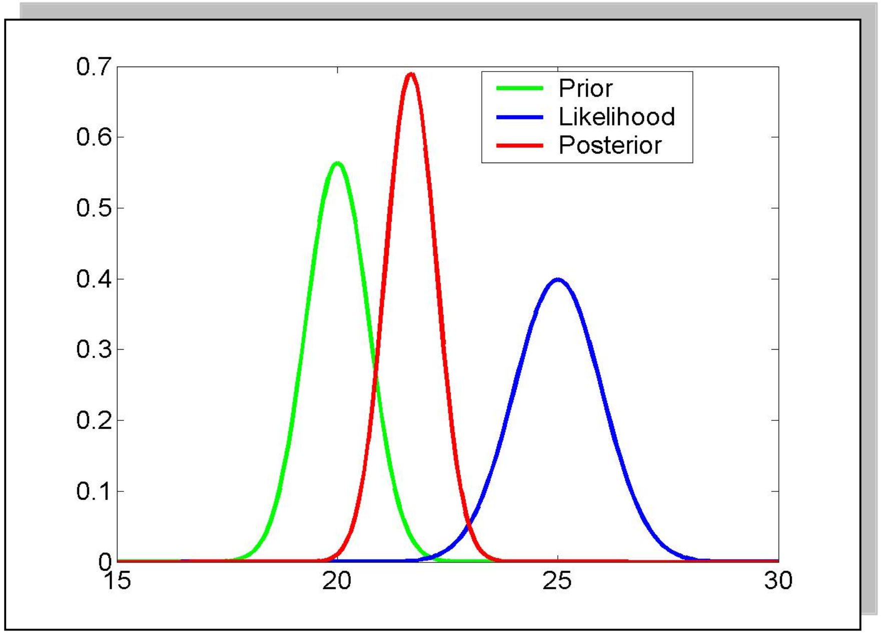
$$p(y\,|\,\theta)$$

prior knowledge

$$p(\theta)$$

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

posterior $\propto$ likelihood • prior



Incorporate **prior knowledge** into computing statistical probabilities.

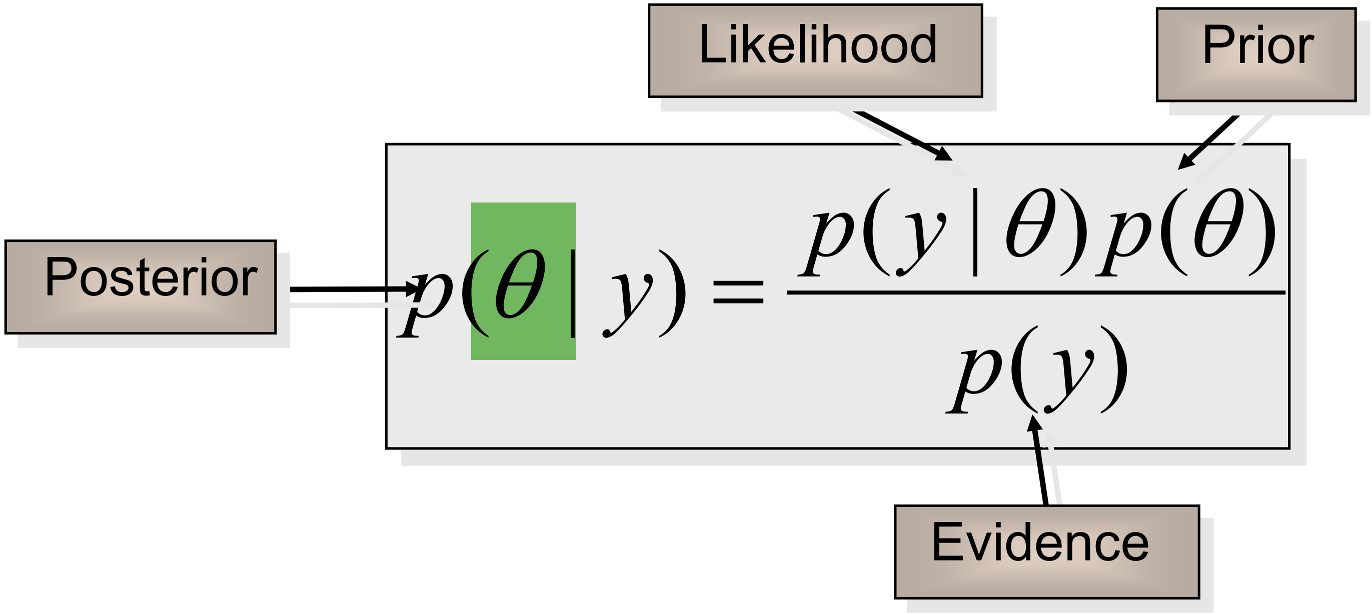
Posterior: combination of prior knowledge and new data, weighted by their relative *precision*

Bayes' rule

Given data *y* and parameters θ, their joint probability can be written as

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

Eliminating *p(y,θ)* gives Bayes' rule:



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

Likelihood

Prior

Posterior

Evidence

Key concepts

- **Prior** probability: the estimate of the probability of the model before the data (evidence) is observed.
- **Posterior** probability: the probability of the model after observing the data (evidence).
- **Likelihood**: the probability of observing a (random) data point given a model (*fixed*) →the compatibility of the data (evidence) with the given model.
- **Marginal likelihood**: "model **evidence**", the same for all possible model variations being considered

Principles of Bayesian inference

⇨ Formulation of a generative model

likelihood $p(y|\theta)$

prior distribution $p(\theta)$

⇨ Observation of data

y

⇨ Update of beliefs based upon observations, given a prior state of knowledge

$$p(\theta \mid y) \propto p(y \mid \theta) p(\theta)$$

Week 6 Contents / Objectives

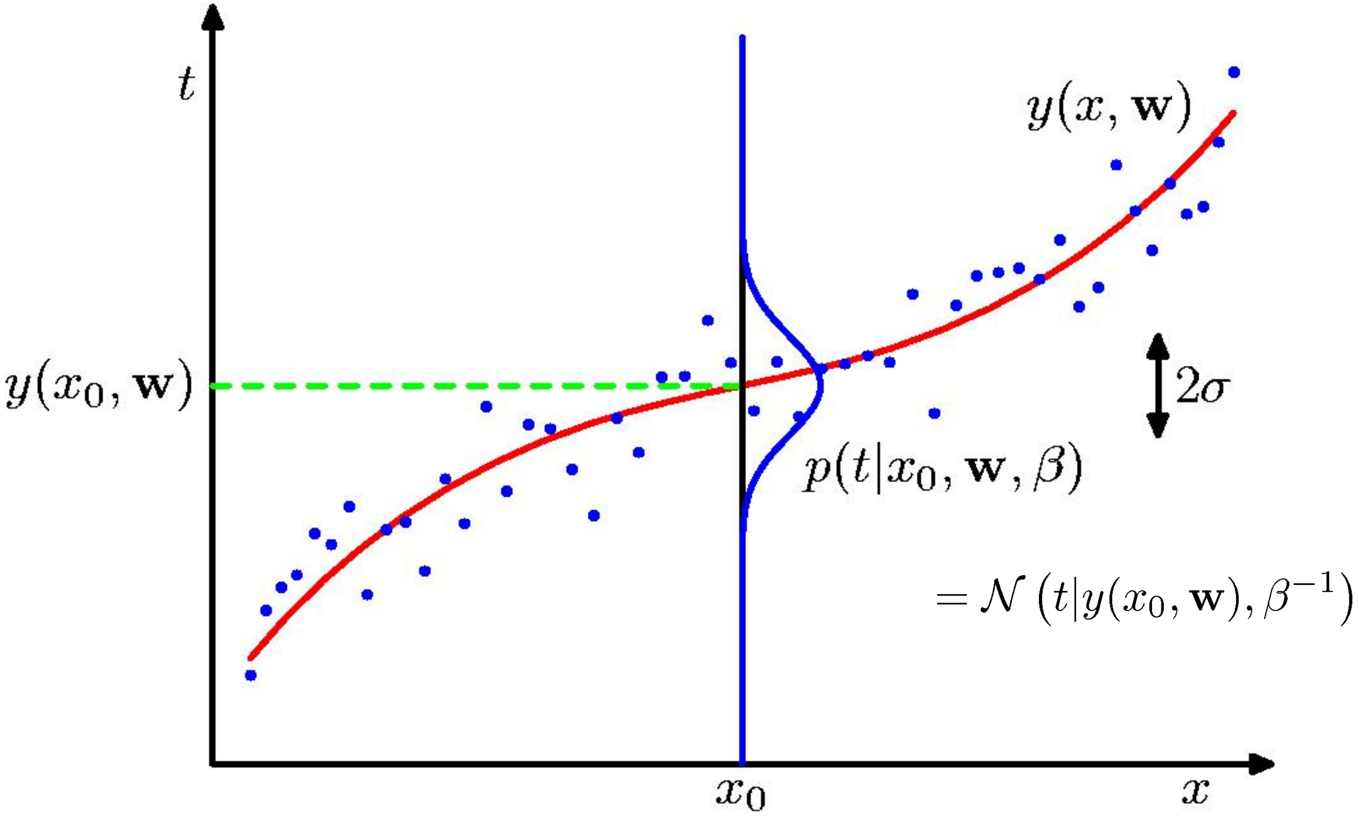
Part A

- Bayesian Inference
- **Bayesian Linear Regression**
- Predictive Distribution

Part B

- Computational Graph
- PyTorch: A Deep Learning Library

Linear Regression: Curve Fitting



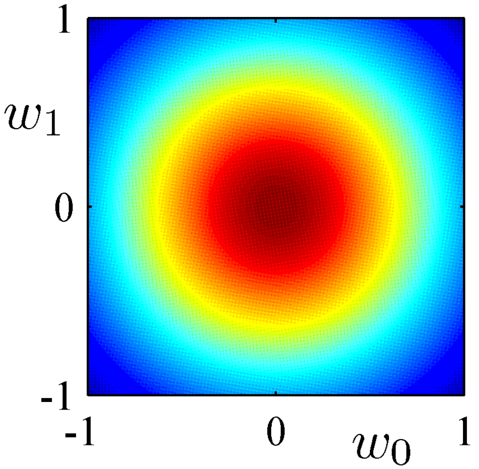
$$= \mathcal{N}\left(t|y(x_0, \mathbf{w}), \beta^{-1}\right)$$

- **Precision** $\beta = \dfrac{1}{\sigma^2}$; note: ***notation difference***

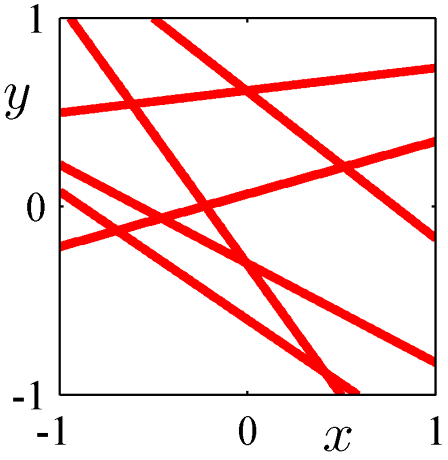
Bayesian Linear Regression (1)

0 data points observed. Six samples of *y(x, **w**)* shown.

Prior

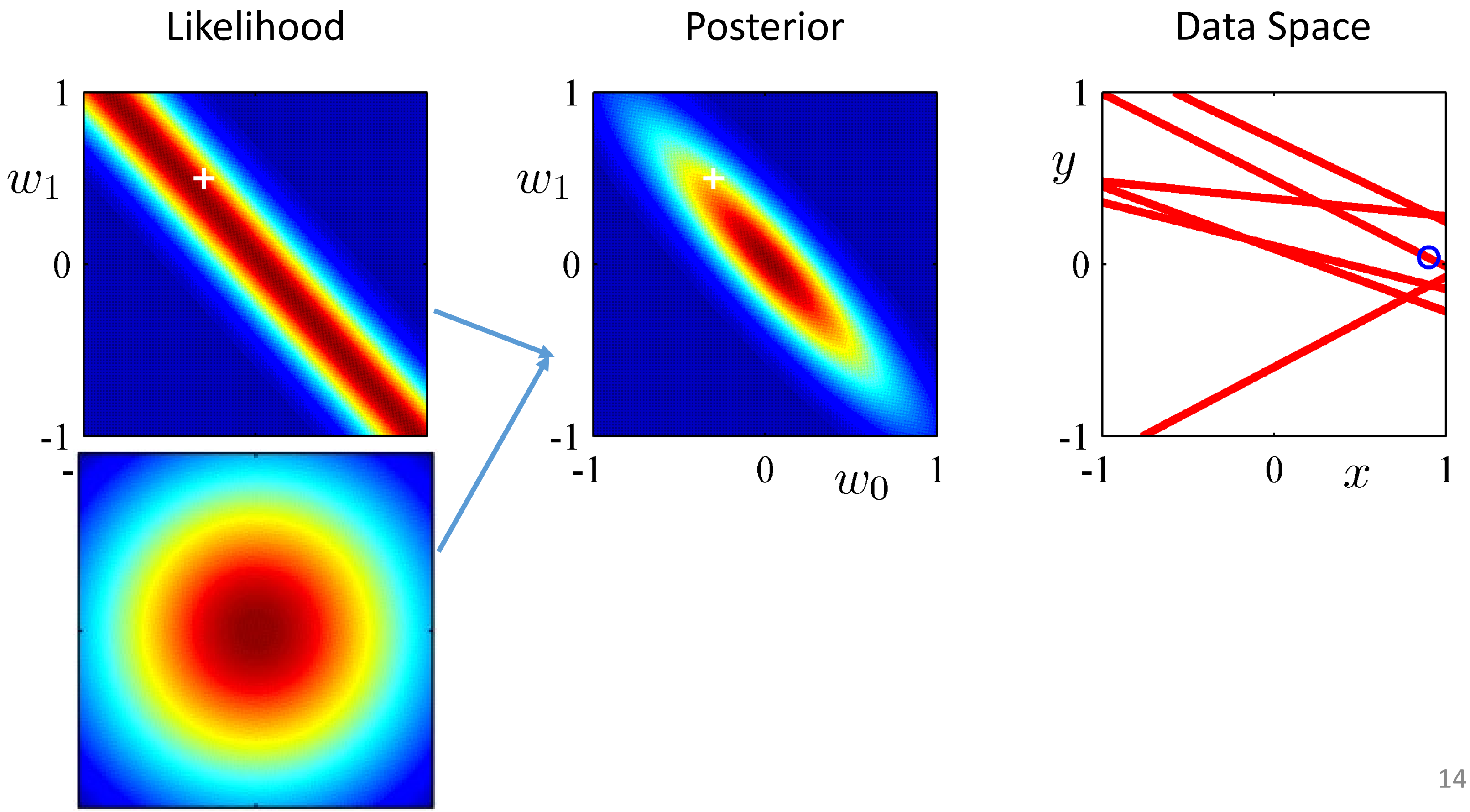


Data Space



Bayesian Linear Regression (2)

1 data point observed → soft constraint. This posterior → prior for the next data point observed)

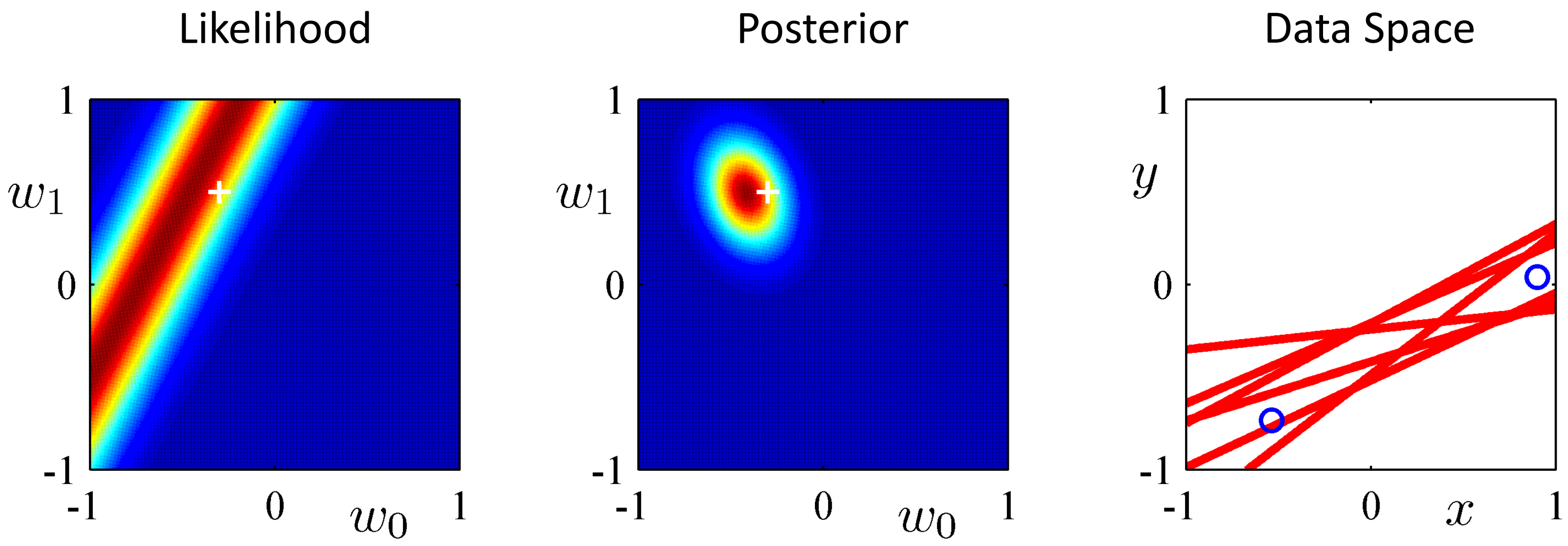

Likelihood

Posterior

Data Space

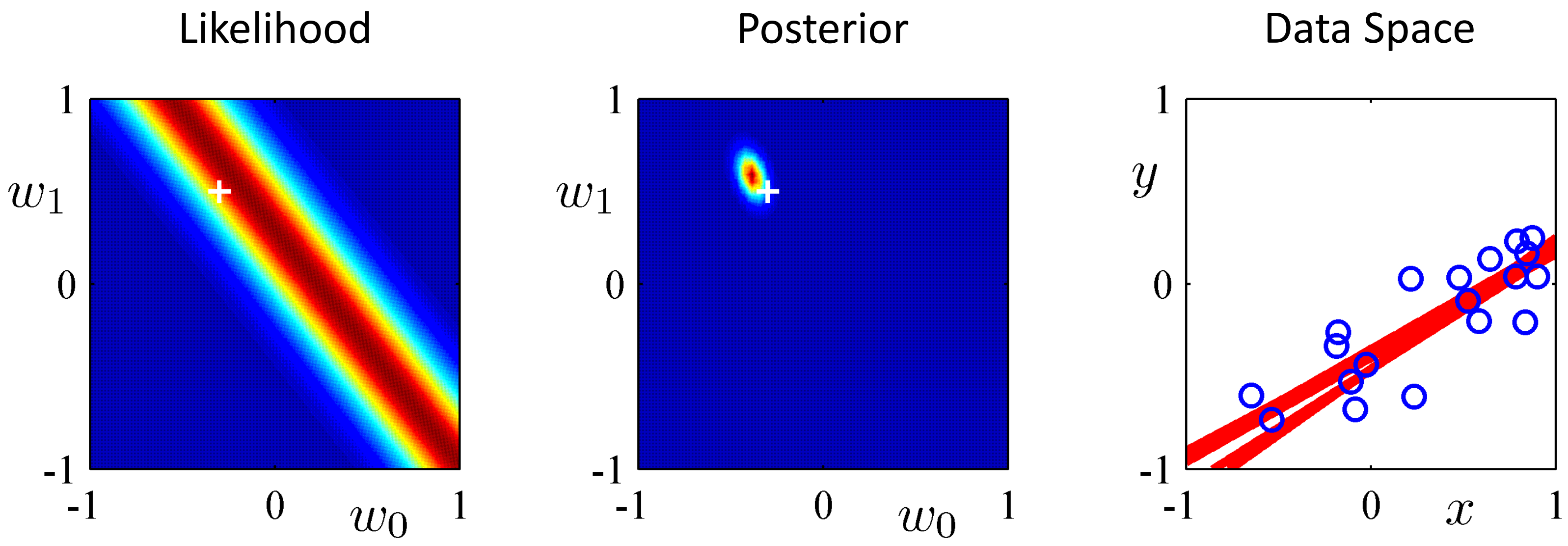
Bayesian Linear Regression (3)

2 data points observed



Bayesian Linear Regression (4)

20 data points observed


Likelihood

Posterior

Data Space

Univariate Gaussian: density est.

Normal densities

$$p(\beta) = N(\beta; \mu_p, \alpha_p^{-1})$$

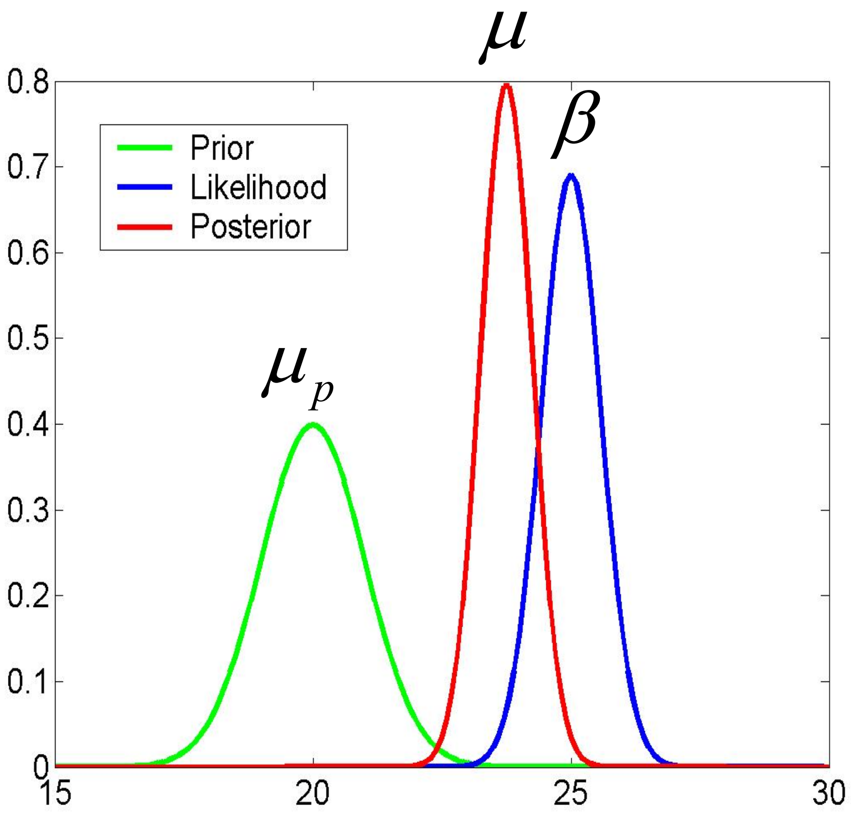
$$p(y \mid \beta) = N(y; \beta, \alpha_e^{-1})$$

$$p(\beta \mid y) = N(\beta; \mu, \alpha^{-1})$$

$$\alpha = \alpha_e + \alpha_p$$

$$\mu = \alpha^{-1}\left(\alpha_e y + \alpha_p \mu_p\right)$$

$$y = \beta + e$$



Posterior mean = precision-weighted combination of prior mean and data mean

Bayesian regression: univariate

Normal densities

$$p(\beta) = N(\beta; \mu_p, \alpha_p^{-1})$$

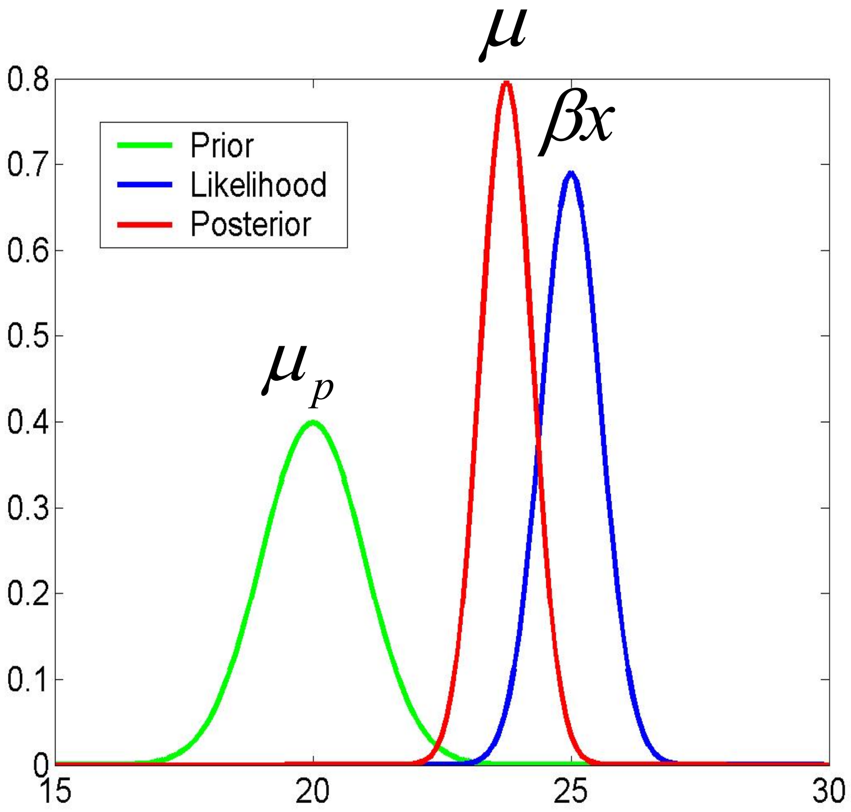
$$p(y \mid \beta) = N(y; \beta x, \alpha_e^{-1})$$

$$p(\beta \mid y) = N(\beta; \mu, \alpha^{-1})$$

$$\alpha = \alpha_e x^2 + \alpha_p$$

$$\mu = \alpha^{-1}\left(\alpha_e x y + \alpha_p \mu_p\right)$$

$$y = \beta x + e$$



Bayesian regression: multivariate

Normal densities

$$p(\beta) = N(\beta; \mu_p, C_p)$$

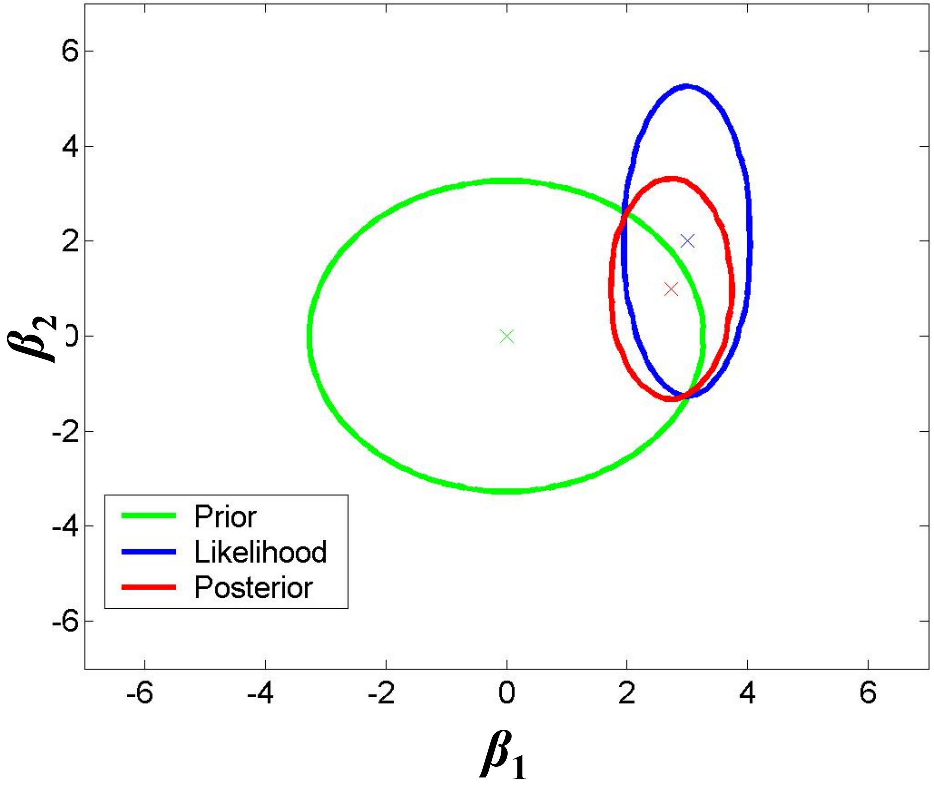
$$p(y \mid \beta) = N(y; X\beta, C_e)$$

$$p(\beta \mid y) = N(\beta; \mu, C)$$

$$C^{-1} = X^T C_e^{-1} X + C_p^{-1}$$

$$\mu = C\left(X^T C_e y + C_p^{-1} \mu_p\right)$$

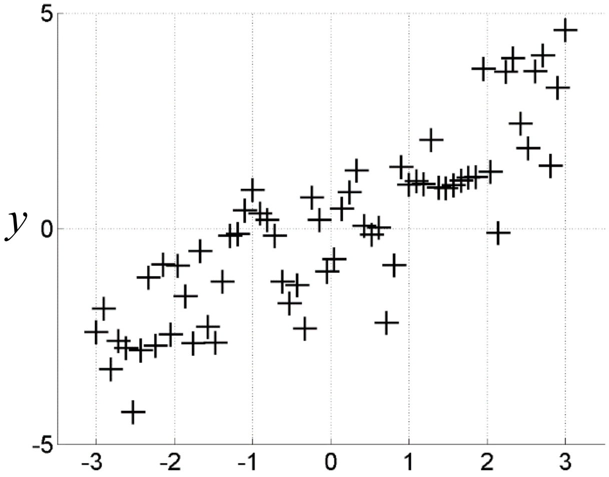
$$y = X\beta + e$$



One step if **C**$_e$ and **C**$_p$ are known. Otherwise iterative estimation (EM).

Linear regression

Data



Ordinary least squares

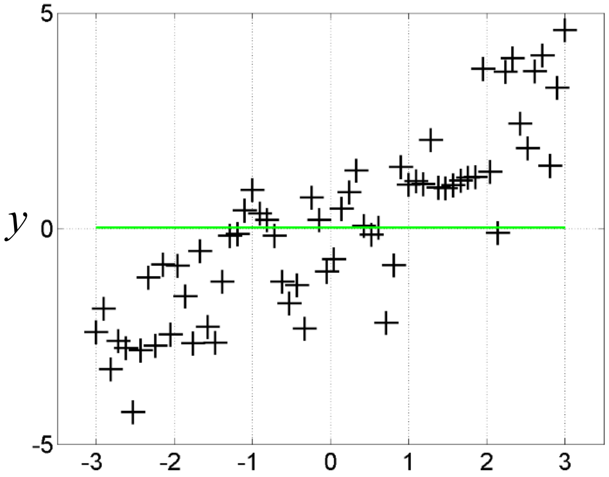
$$y = X\beta$$

$$E_D = (y - X\beta)^T (y - X\beta)$$

$$\frac{\partial E_D}{\partial \beta} = 0 \Rightarrow \hat{\beta}_{ols} = (X^T X)^{-1} X^T y$$

Linear regression

Data and model fit



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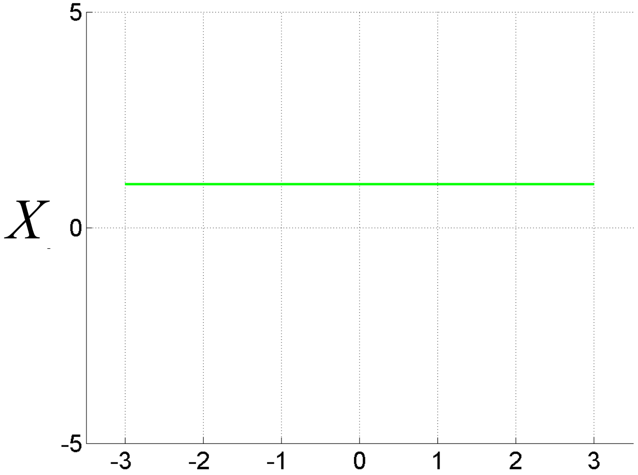
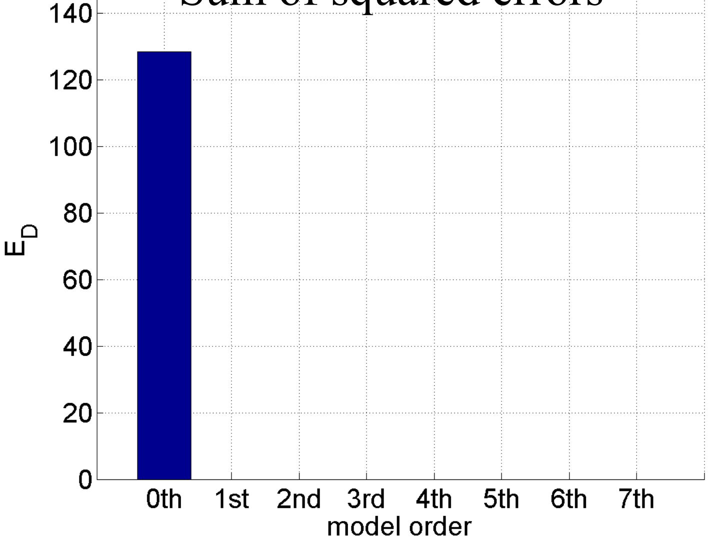
Bases (explanatory variables)

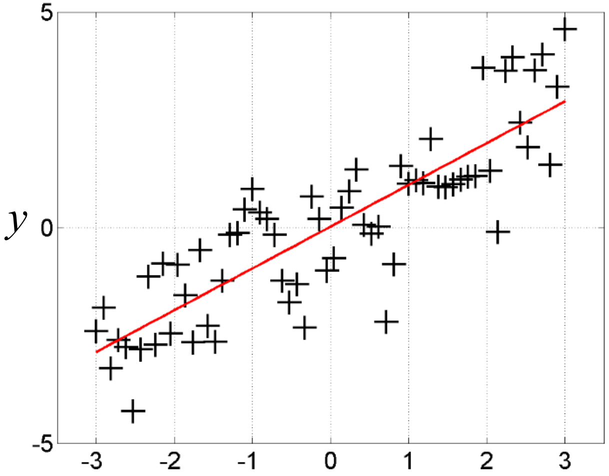


Sum of squared errors



Linear regression

Data and model fit



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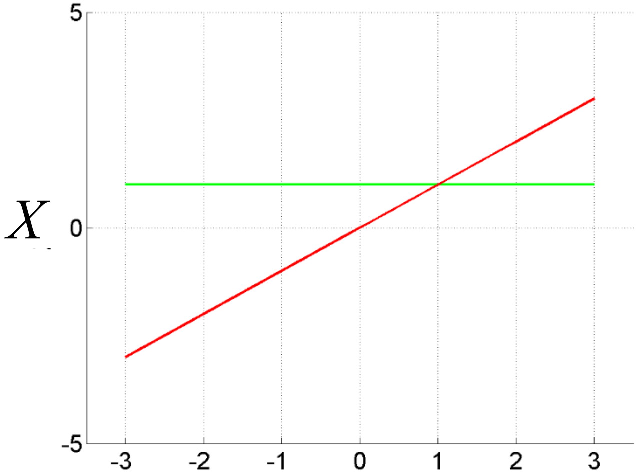

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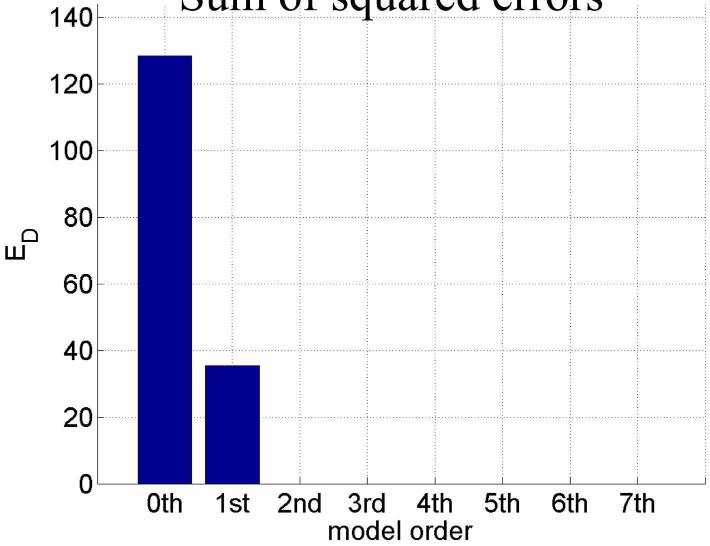
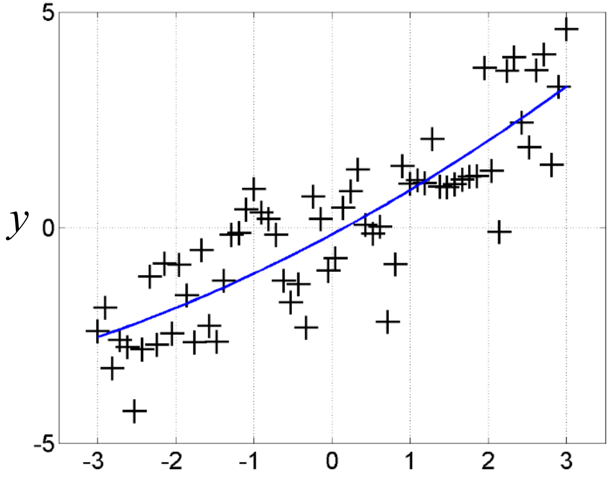


Linear regression

Data and model fit



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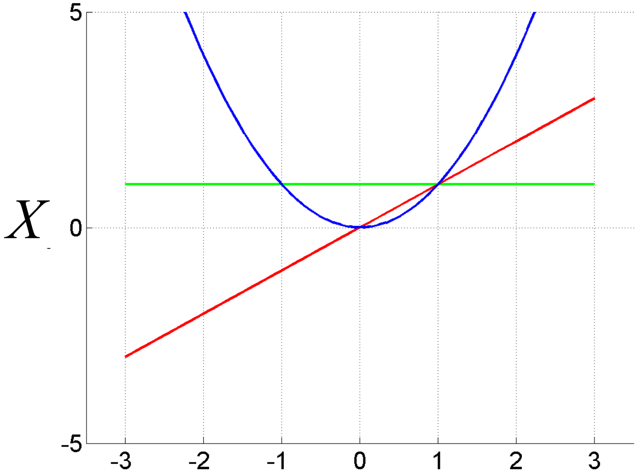

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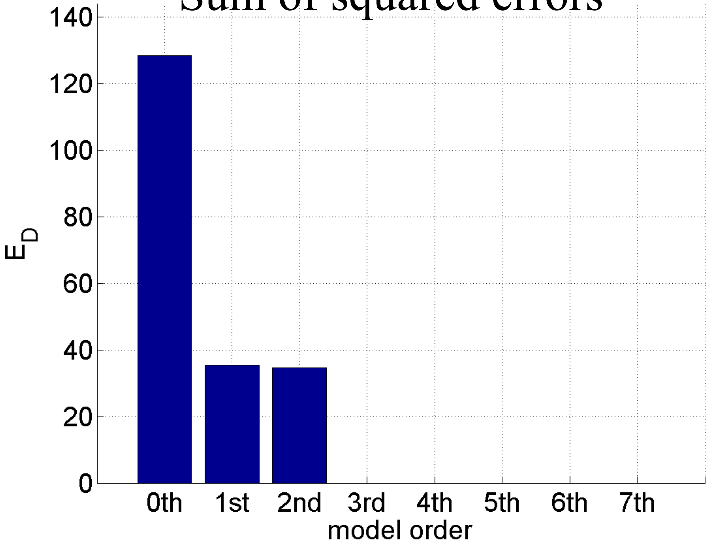
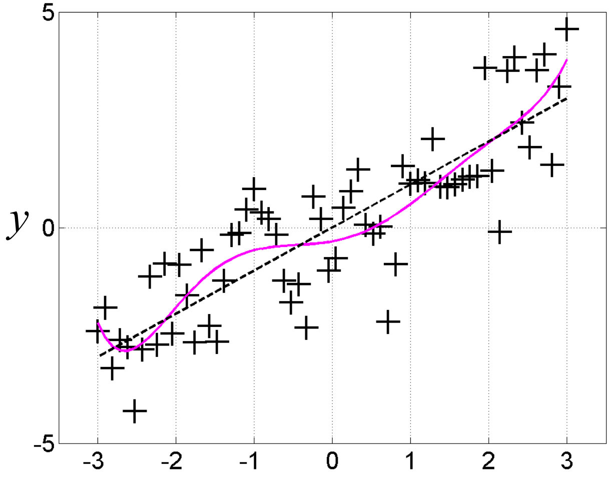


Linear regression

Data and model fit

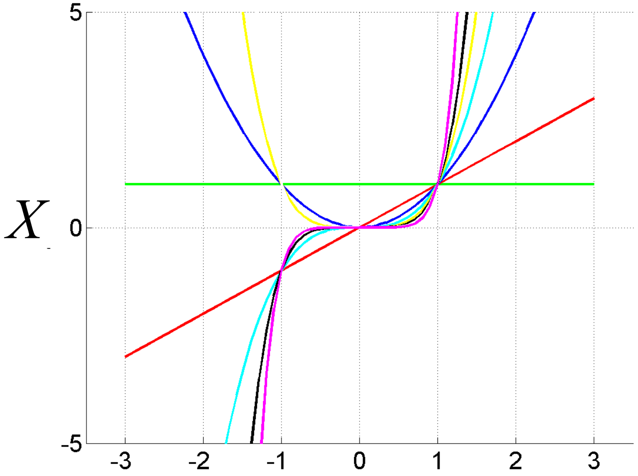


Ordinary least squares

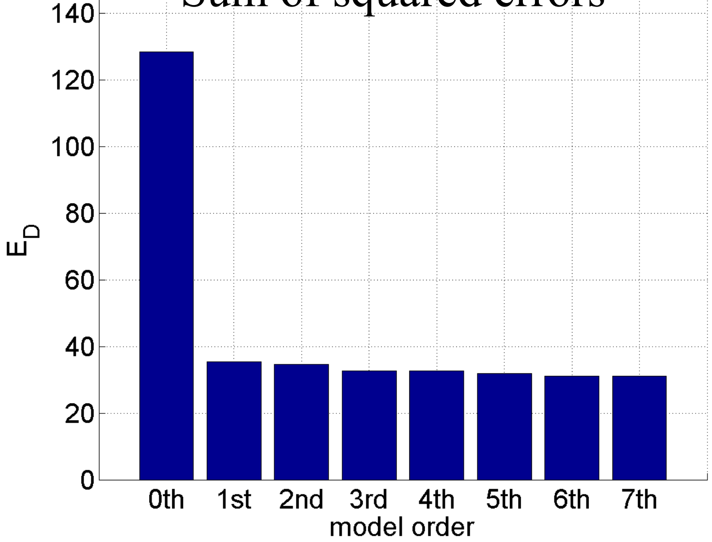
Over-fitting: model fits noise

Solution: include uncertainty in model parameters

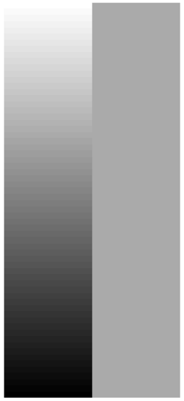
Bases (explanatory variables)



Sum of squared errors

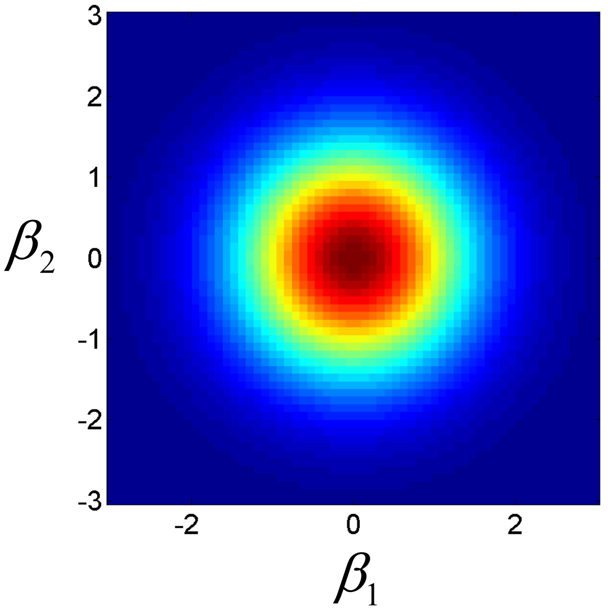


Bayesian regression: *priors & likelihood*

$X =$ 

Model: $y = X\beta + e$

Bayesian regression: *priors & likelihood*

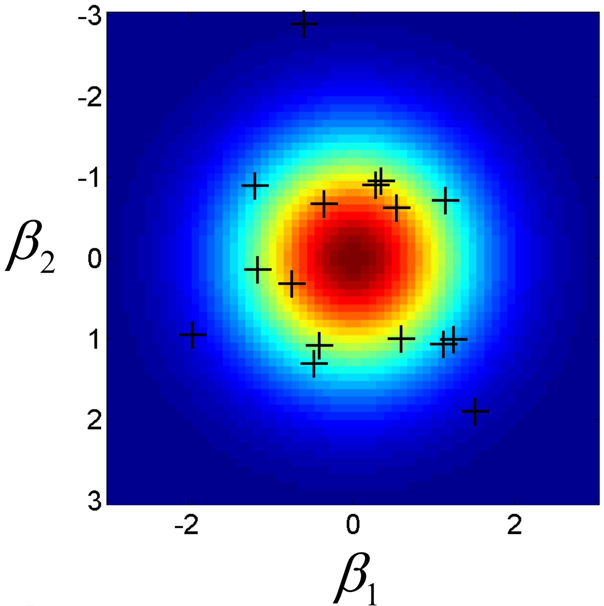


Model: $$y = X\beta + e$$

Prior: $$p(\beta|\alpha_2) = N_k(0, \alpha_2^{-1} I_k)$$

$$\propto \exp(-\alpha_2 \|\beta\|^2 / 2)$$

Bayesian regression: *priors & likelihood*



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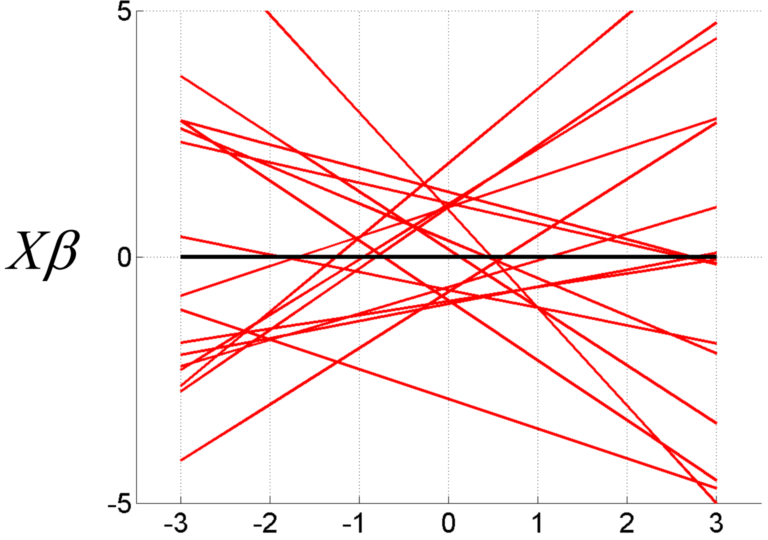
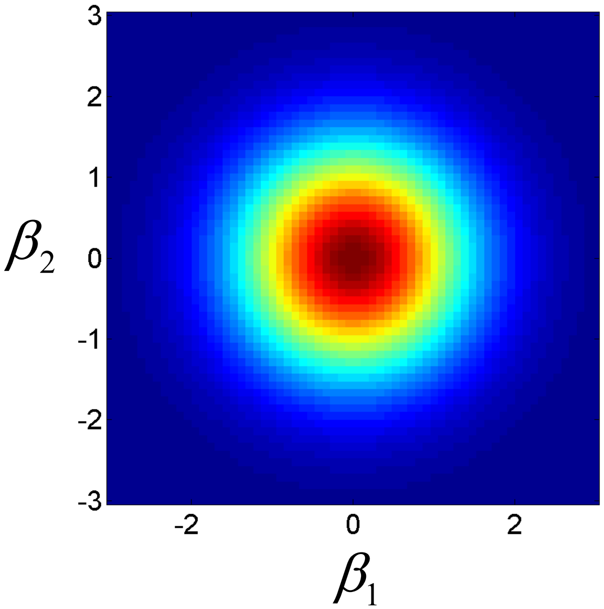


🟥 Sample curves from prior (before observing any data)

▬ Mean curve

Bayesian regression: *priors & likelihood*



Model: $y = X\beta + e$

Prior: $p(\beta|\alpha_2) = N_k(0, \alpha_2^{-1} I_k)$

$$\propto \exp(-\alpha_2 \|\beta\|^2 / 2)$$

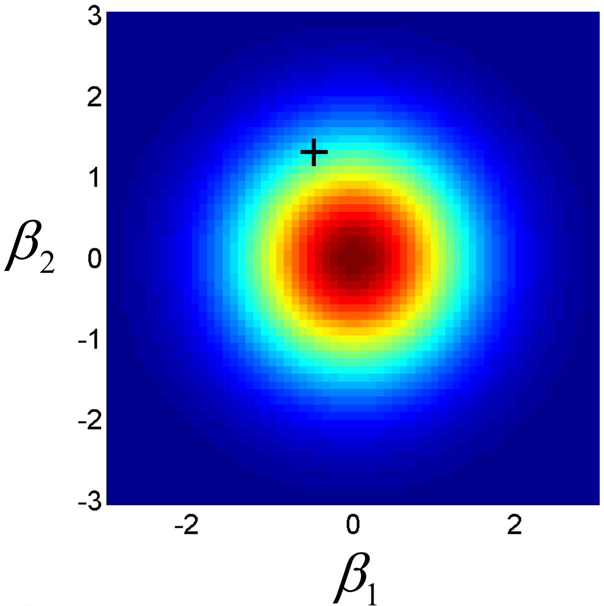
Likelihood:

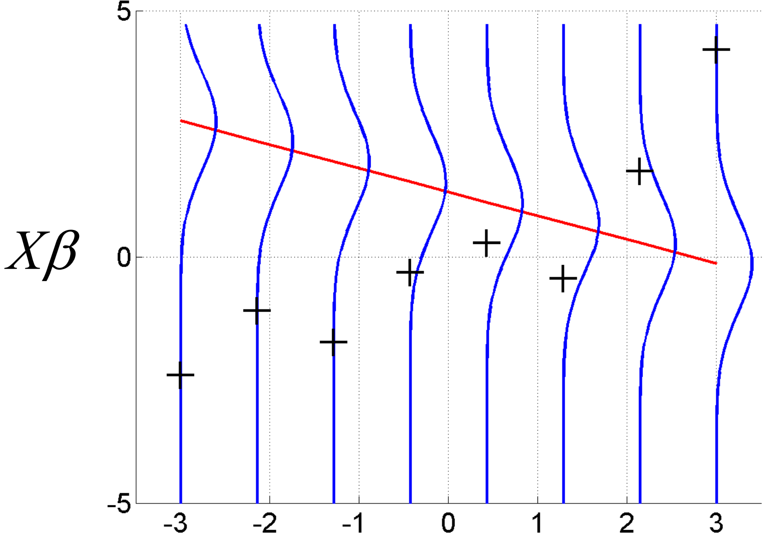
$$p(y|\beta, \alpha_1) = \prod_{i=1}^{N} p(y_i \mid \beta, \alpha_1^{-1})$$

$$p(y_i|\beta, \alpha_1) = N(X_i\beta, \alpha_1^{-1})$$

$$\propto \exp(-\alpha_1 (y_i - X_i\beta)^2 / 2)$$

Bayesian regression: *priors & likelihood*





Model: $$y = X\beta + e$$

Prior: $$p(\beta|\alpha_2) = N_k(0, \alpha_2^{-1} I_k)$$
$$\propto \exp(-\alpha_2 \|\beta\|^2 / 2)$$

Likelihood:
$$p(y|\beta, \alpha_1) = \prod_{i=1}^{N} p(y_i \mid \beta, \alpha_1^{-1})$$
$$p(y_i|\beta, \alpha_1) = N(X_i \beta, \alpha_1^{-1})$$
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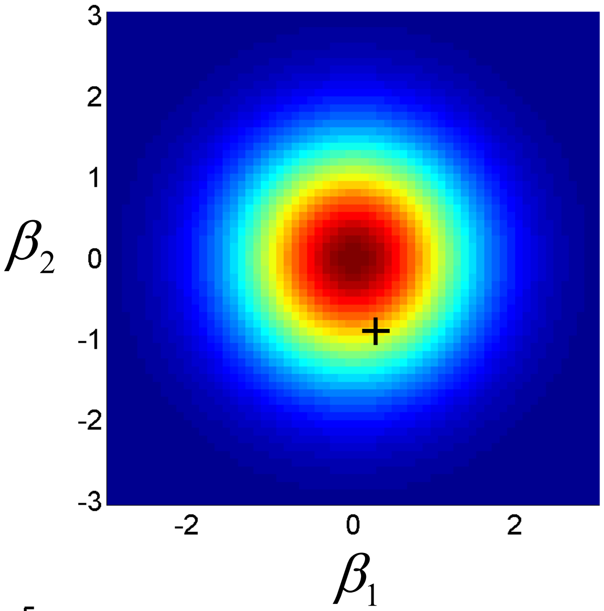
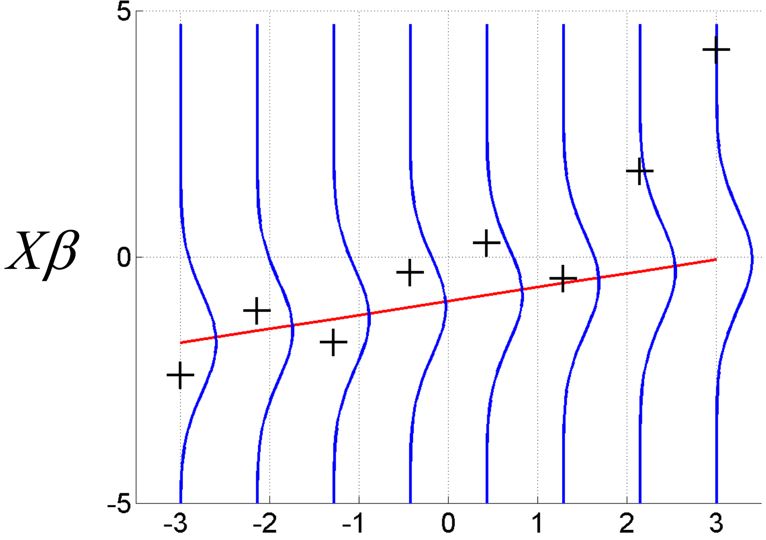
Bayesian regression: *priors & likelihood*





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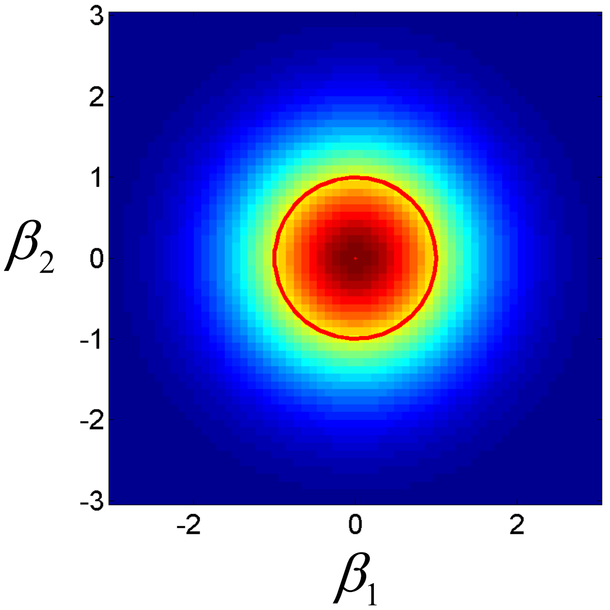
$$p(y_i|\beta, \alpha_1) = N(X_i \beta, \alpha_1^{-1})$$

$$\propto \exp(-\alpha_1 (y_i - X_i \beta)^2 / 2)$$

Bayesian regression: *posterior*



Model: $y = X\beta + e$

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$$\propto \exp(-\alpha_2 \|\beta\|^2 / 2)$$

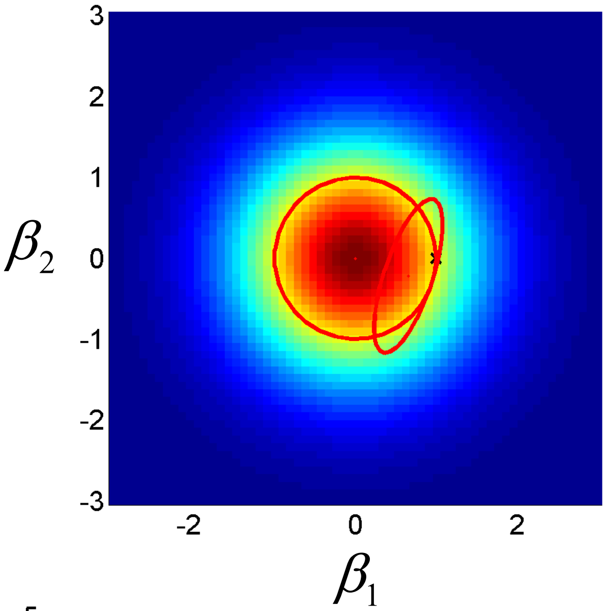
Likelihood:

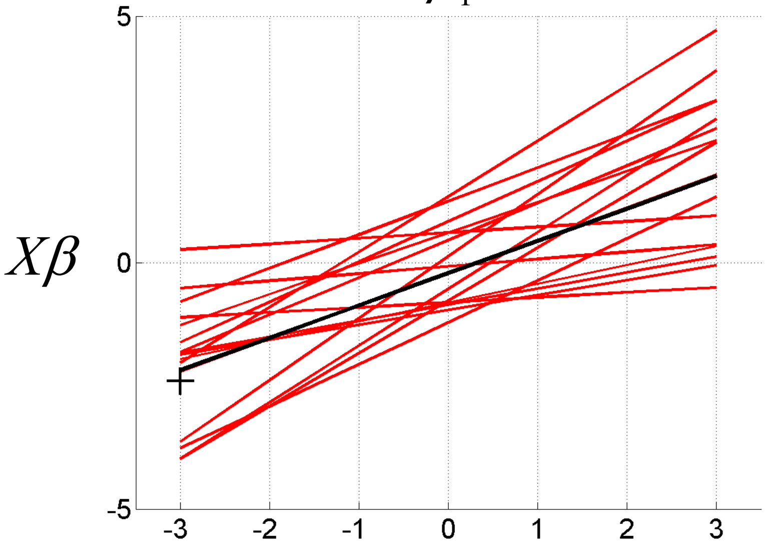
$$p(y|\beta,\alpha_1) = \prod_{i=1}^{N} p(y_i \mid \beta, \alpha_1)$$

Bayes Rule:

$$p(\beta|y,\alpha) \propto p(y \mid \beta, \alpha)\, p(\beta \mid \alpha)$$

Bayesian regression: *posterior*





Model:

$$y = X\beta + e$$

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$$\propto \exp(-\alpha_2 \|\beta\|^2 / 2)$$

Likelihood:

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Bayes Rule:

$$p(\beta | y, \alpha) \propto p(y \mid \beta, \alpha) p(\beta \mid \alpha)$$

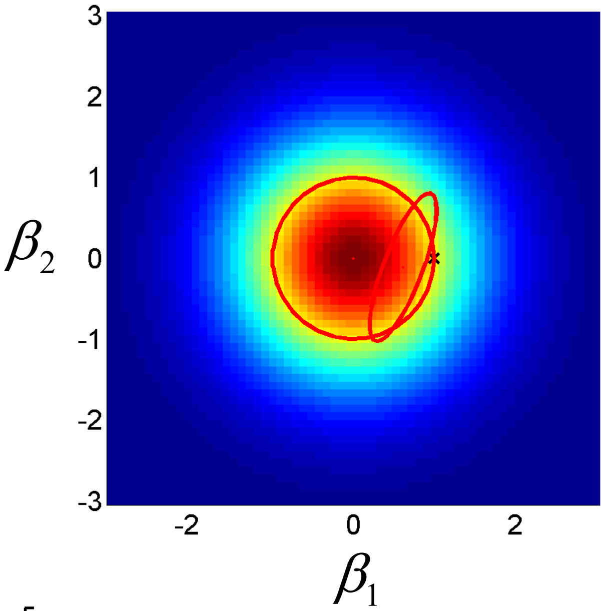
Posterior:

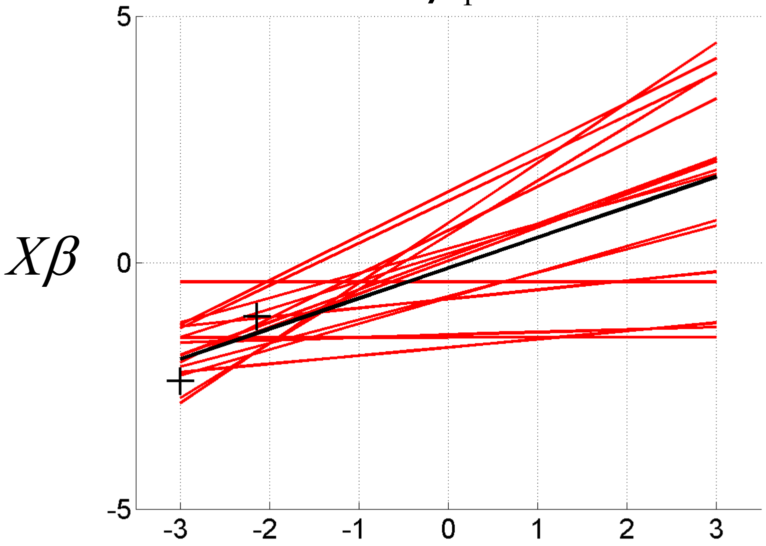
$$p(\beta \mid y, \alpha) = N(\mu, C)$$

$$C = (\alpha_1 X^T X + \alpha_2 I_k)^{-1}$$

$$\mu = \alpha_1 C X^T y$$

Bayesian regression: *posterior*





Model: $$y = X\beta + e$$

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Posterior: $$p(\beta \mid y, \alpha\ ) = N(\mu, C)$$
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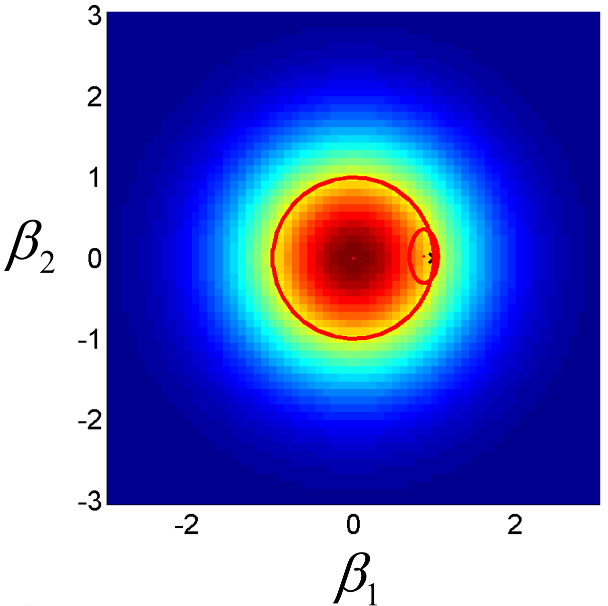
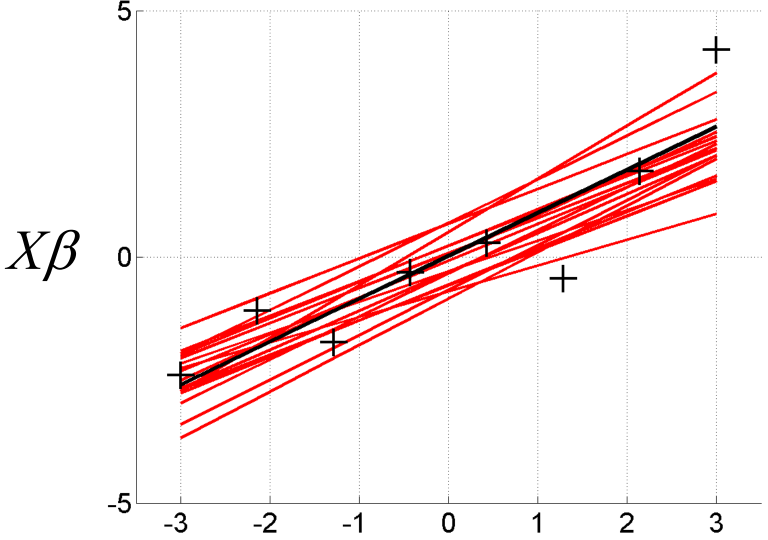
Bayesian regression: *posterior*





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Bayes Rule:
$$p(\beta|y, \alpha) \propto p(y \mid \beta, \alpha) p(\beta \mid \alpha)$$

Posterior:
$$p(\beta \mid y, \alpha\ ) \ = N(\mu, C)$$
$$C = \left(\alpha_1 X^T X + \alpha_2 I_k\right)^{-1}$$
$$\mu = \alpha_1 C X^T y$$

Question

$$p(\beta \mid y, \alpha) = N(\mu, C)$$

$$C = \left(\alpha_1 X^T X + \alpha_2 I_k\right)^{-1}$$

$$\mu = \alpha_1 C X^T y$$

- What is the point estimate for the model parameter beta from the above?

Maximum A Posteriori

Week 6 Contents / Objectives

Part A

- Bayesian Inference
- Bayesian Linear Regression
- **Predictive Distribution**

Part B

- Computational Graph
- PyTorch: A Deep Learning Library

MAP vs MLE

- MAP: Maximum A Posteriori

$$\boldsymbol{\beta}^* = \boldsymbol{\mu} = \alpha_1 \left[\alpha_1 \mathbf{X}^\top \mathbf{X} + \alpha_2 \mathbf{I}_k\right]^{-1} \mathbf{X}^\top \mathbf{y}$$

$$\boldsymbol{\beta}^* = \boldsymbol{\mu} = \left[\mathbf{X}^\top \mathbf{X} + \frac{\alpha_2}{\alpha_1} \mathbf{I}_k\right]^{-1} \mathbf{X}^\top \mathbf{y}$$

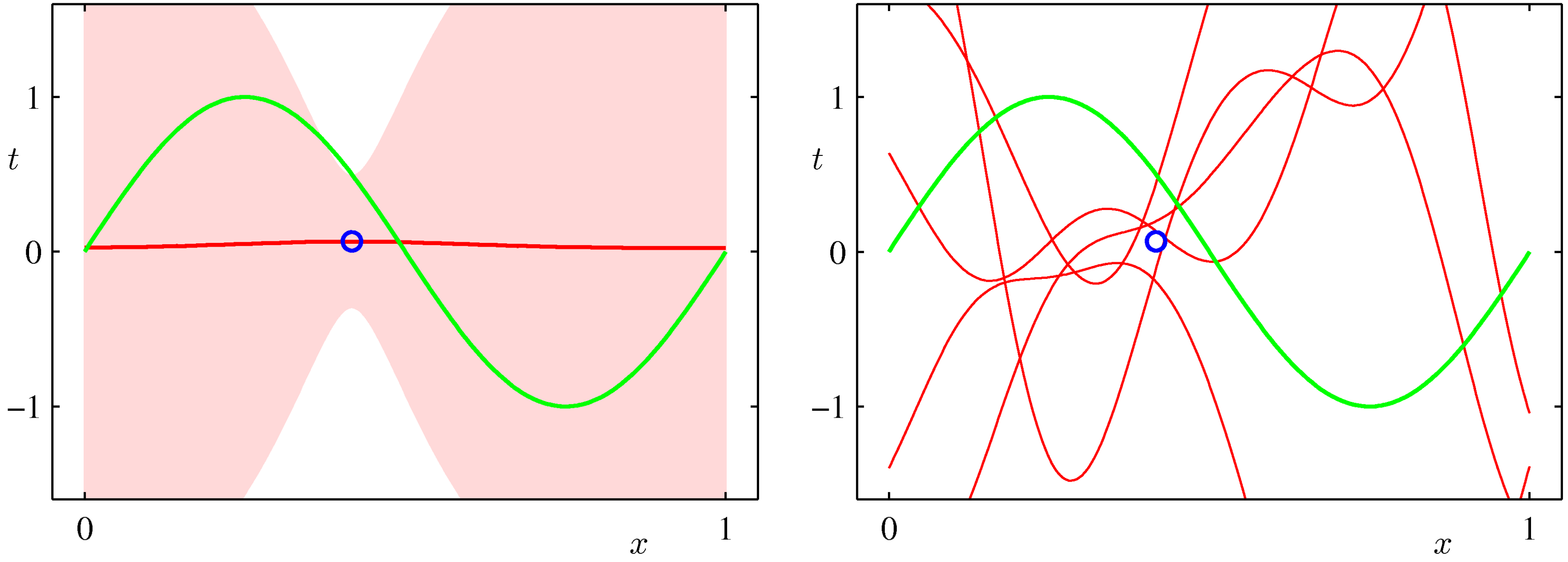
- MLE: Maximum Likelihood Estimation

$$\boldsymbol{\beta}^* = \left[\mathbf{X}^\top \mathbf{X} + \mathbf{I}_k\right]^{-1} \mathbf{X}^\top \mathbf{y}$$

- MAP = regularised MLE

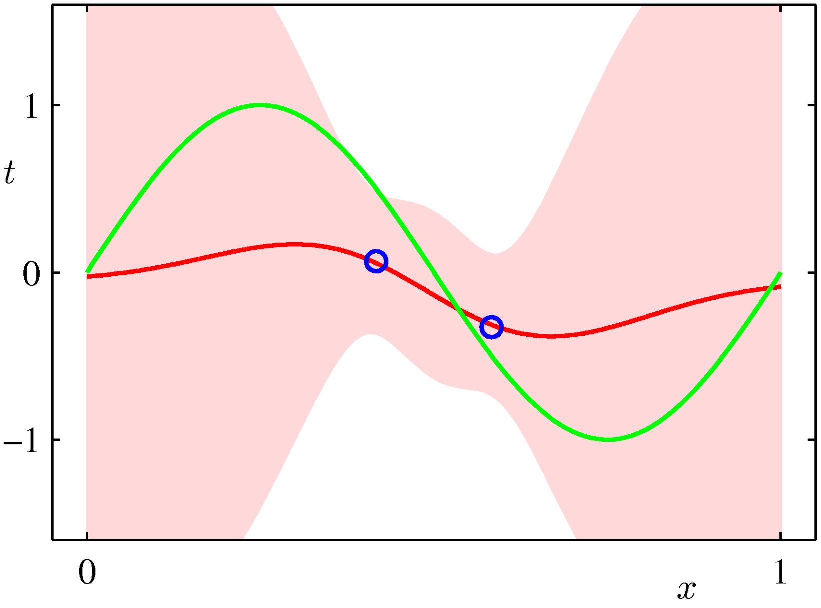
Predictive Distribution (1)

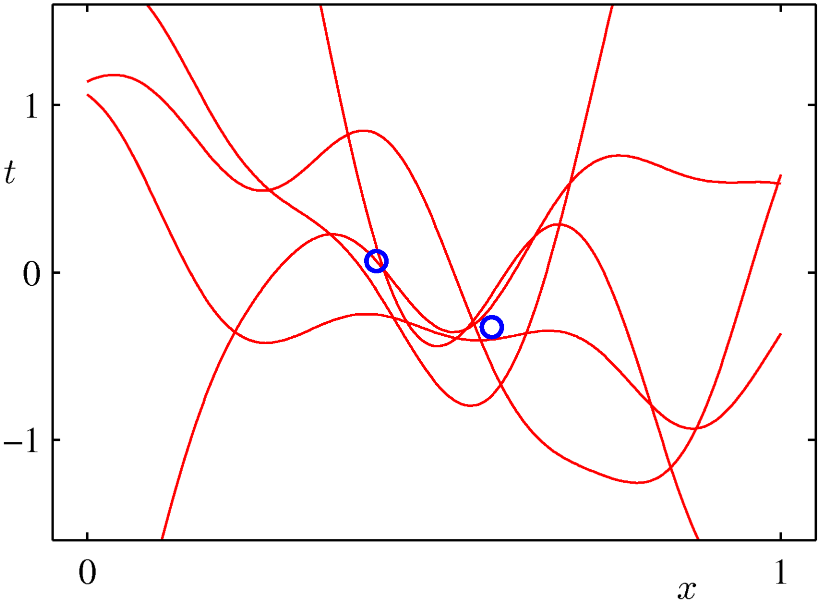
- Example: Sinusoidal data, 9 Gaussian basis functions, 1 data point



Predictive Distribution (2)

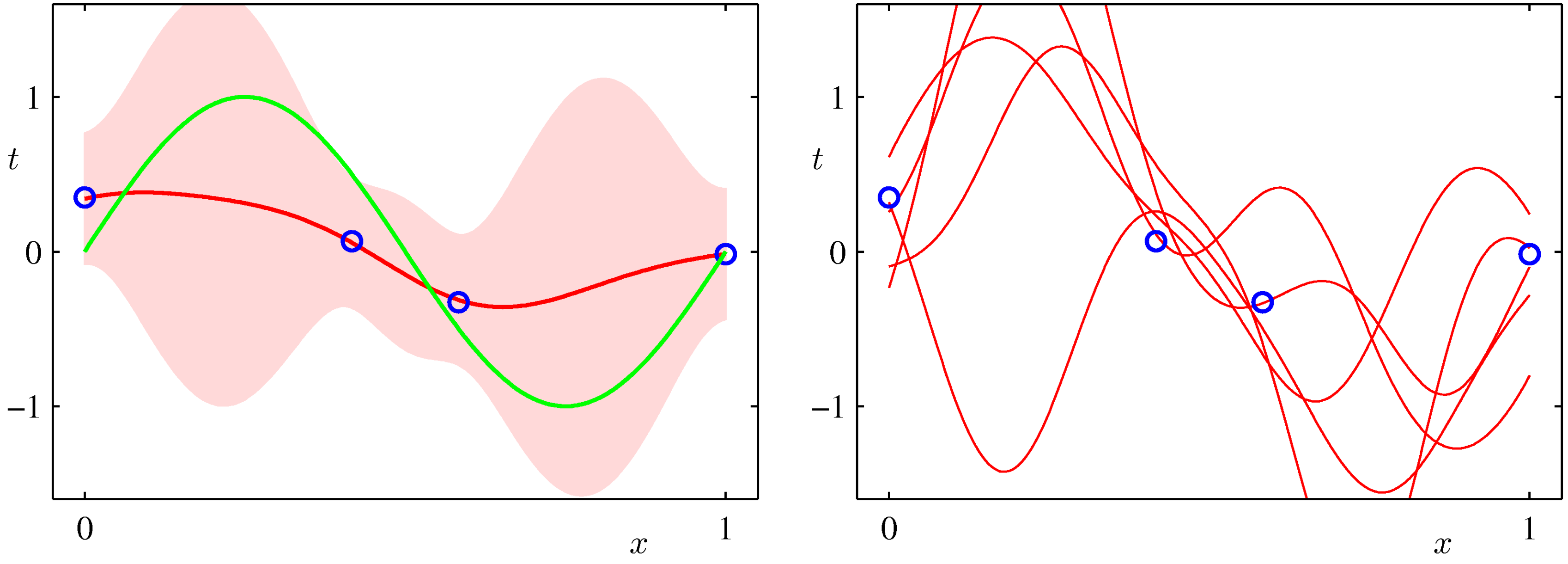
- Example: Sinusoidal data, 9 Gaussian basis functions, 2 data points





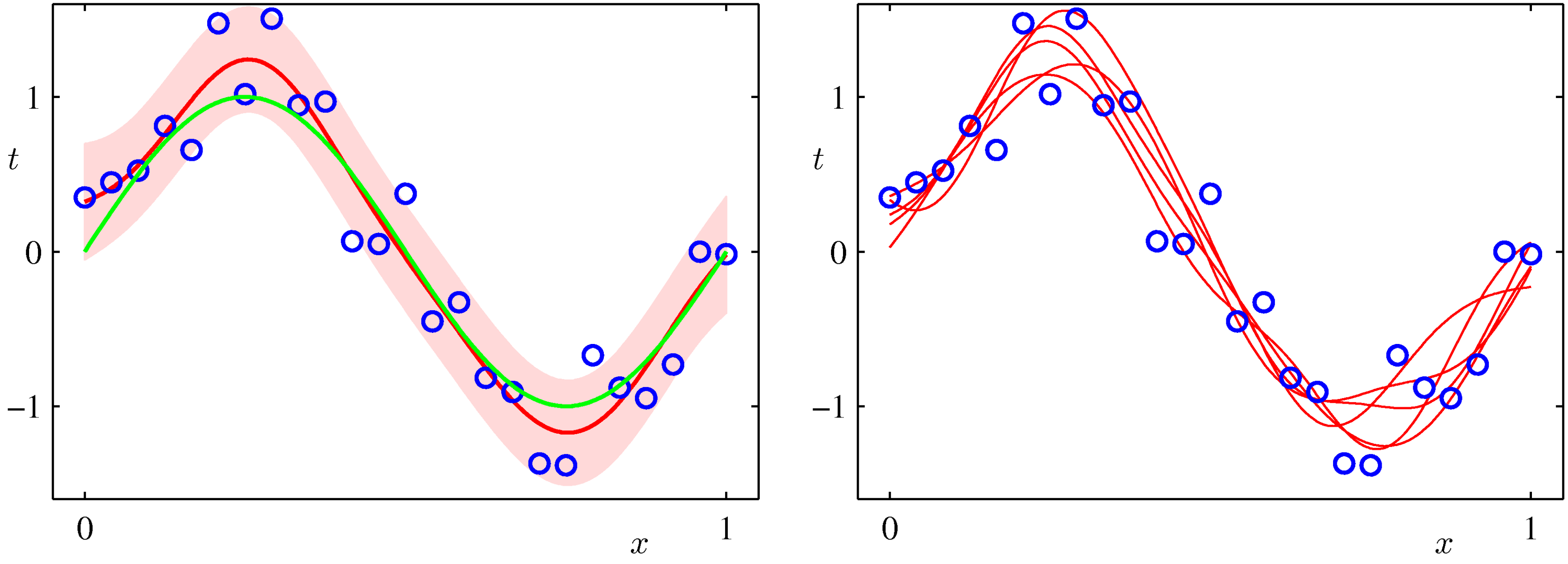
Predictive Distribution (3)

- Example: Sinusoidal data, 9 Gaussian basis functions, 4 data points



Predictive Distribution (4)

- Example: Sinusoidal data, 9 Gaussian basis functions, 25 data points



- Notice the decreased uncertainty

Pros and Cons of Bayesian

- Advantages
  - Deal with uncertainty.
  - Make use of more information (prior, if available)
  - Less overfitting in general

- Disadvantages
  - Complexity
  - Subjectivity: all inferences are based on beliefs. Which prior to choose?

Summary on Bayesian regression

- Bayesian inference: placing a probability distribution (prior density) over the model parameters for their probabilistic interpretation
- Bayesian regression: Bayesian treatment of linear regression (model parameters)
- Key Bayesian concepts: prior, posterior, likelihood, marginal likelihood, Bayes' rule, marginalisation

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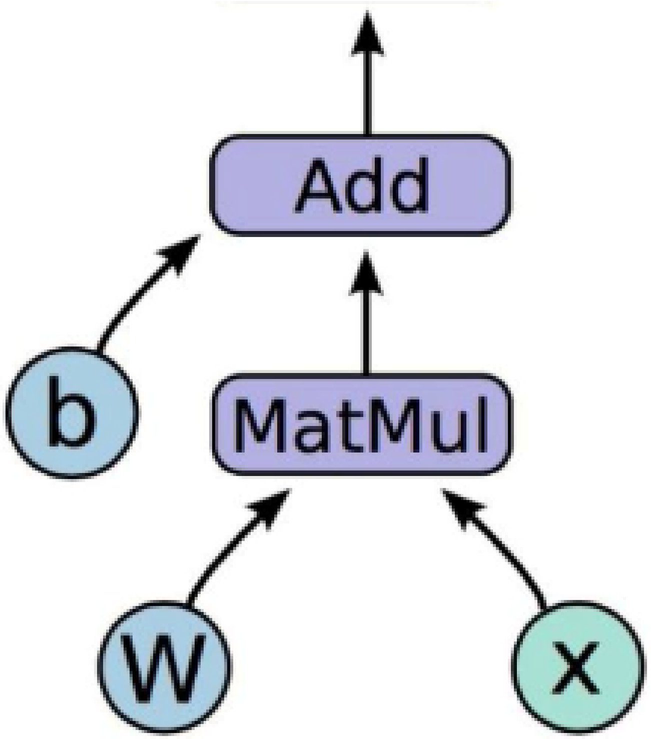
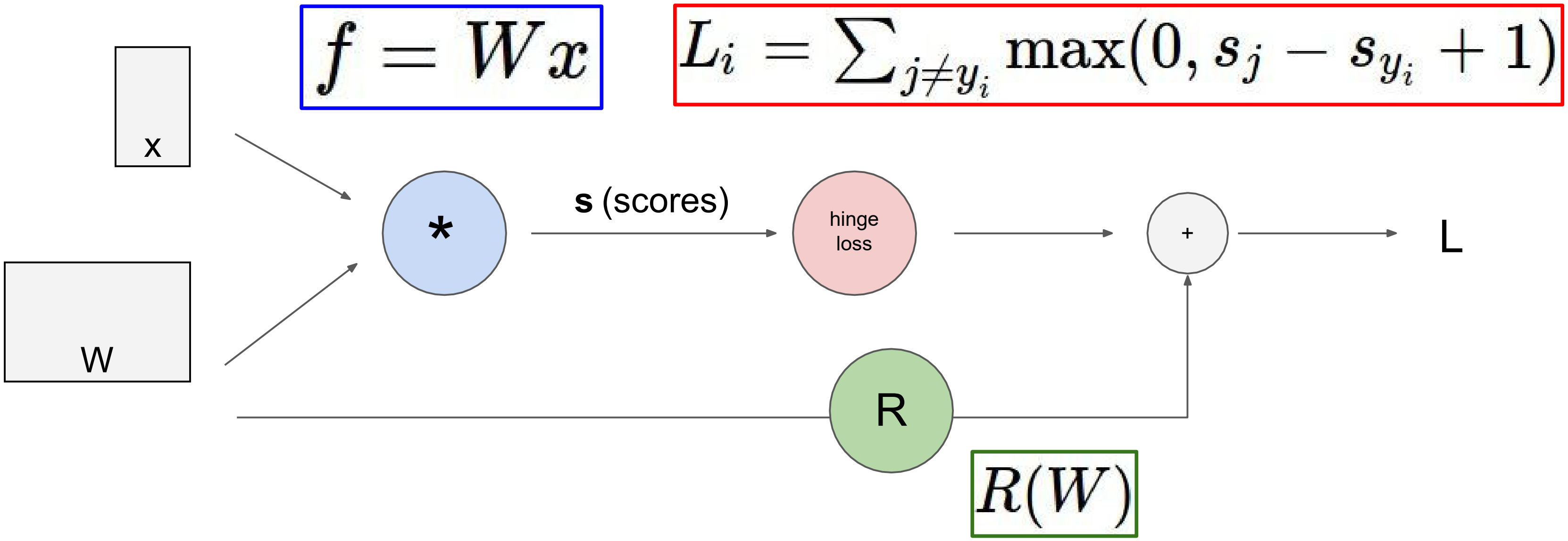
Computational Graph: L Regression

- Linear regression $\mathbf{y} = \mathbf{W}\mathbf{x} + \mathbf{b}$



Source: Nelson Liu: https://colab.research.google.com/drive/11iLtGFDpnIuHj5B0rQDGG5lqq6BQ8FRh

Computational Graph: w/t Reg.

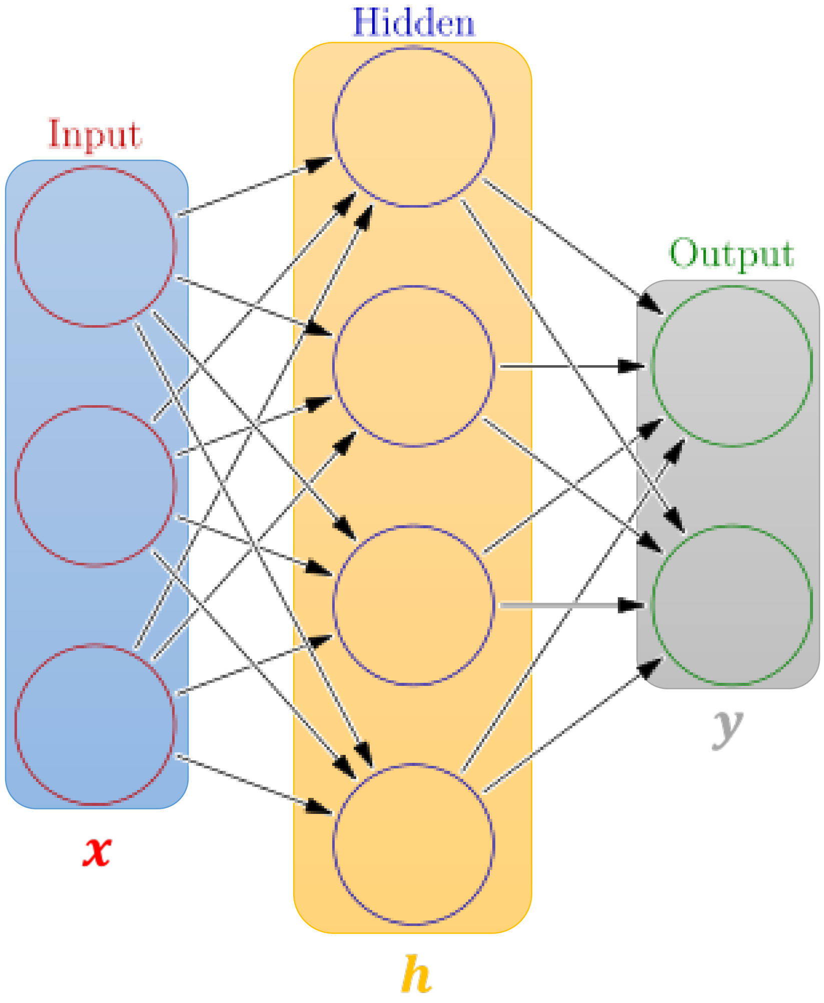


$$f = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

$$R(W)$$

Multilayer Perceptron (NN) vs LR



Weights

$$h = \sigma(W_1 x + b_1)$$

$$y = \sigma(W_2 h + b_2)$$

Activation functions

Question:

How many model parameters?

[3 x 4] + [4 x 2] = 20 weights

4 + 2 = 6 biases

26 learnable **parameters**

4 + 2 = 6 neurons (not counting inputs)

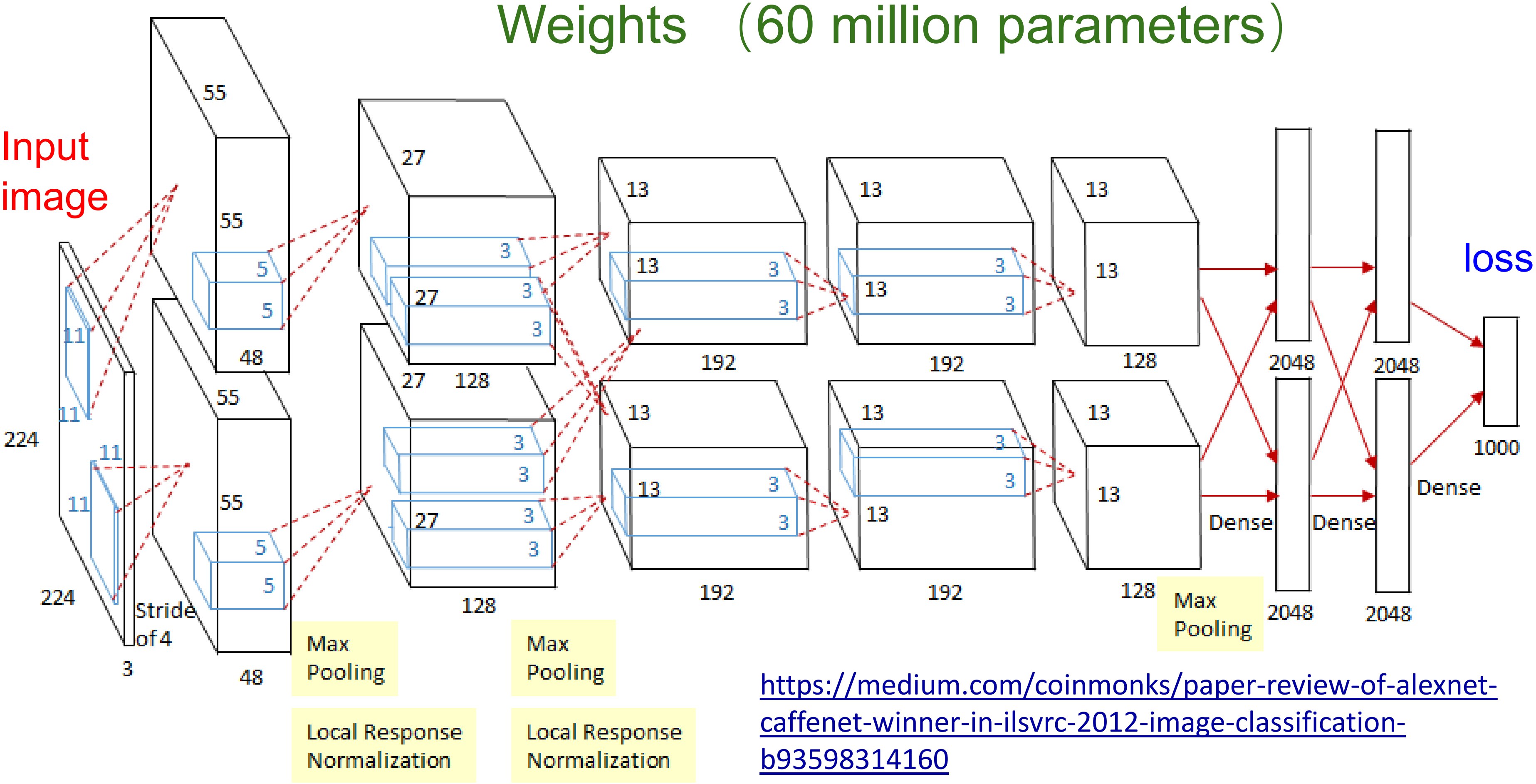
Source: https://miro.medium.com/max/570/0*y8AuUHSoTGRqX40h.jpeg

Computational Graph: DL

Weights （60 million parameters）

Input image

loss



https://medium.com/coinmonks/paper-review-of-alexnet-caffenet-winner-in-ilsvrc-2012-image-classification-b93598314160

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- **PyTorch: A Deep Learning Library**

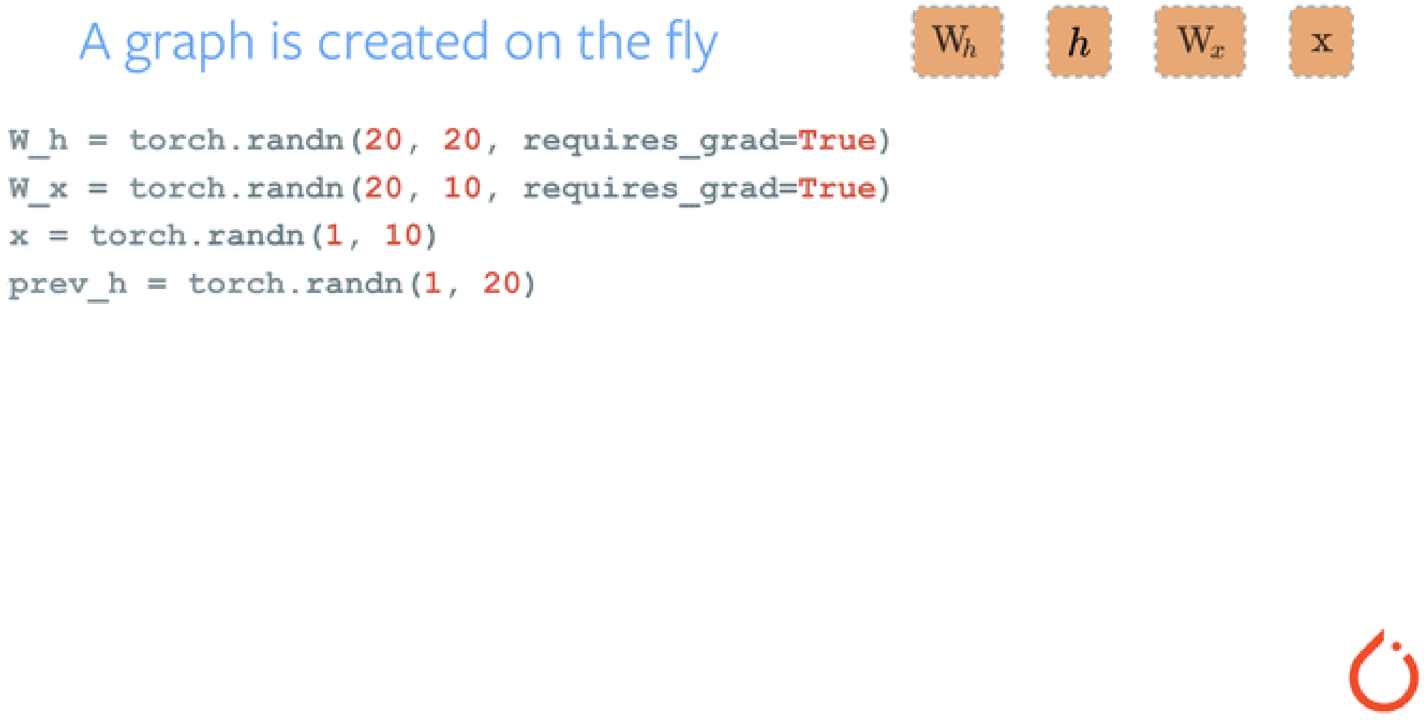
PyTorch

- An open source deep learning library by Facebook
  - **Tensor** computing (like NumPy) with strong acceleration via graphics processing units (GPU)
  - Deep neural networks built on a tape-based autodiff system
- **torch.Tensor**
  - multidimensional array data structures (arrays) for programming
  - Scalar: 0D tensor
  - Vector: 1D tensor
  - Matrix: 2D tensor

Key Modules in PyTorch

- **torch.autograd**
  - Automatic differentiation. A recorder records what operations have performed, and then it replays it backward to compute the gradients.
- **torch.optim**
  - Implementation of various optimization algorithms used for building neural networks (and other ML algorithms).
- **torch.nn**
  - High-level definition of the **computational graphs** of complex neural networks (and other ML algorithms)

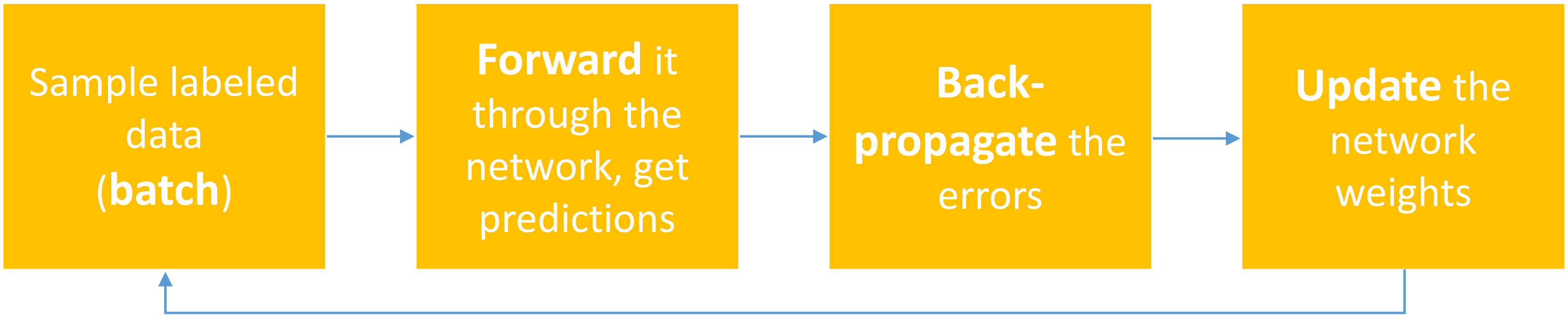
Dynamic Computational Graph



A graph is created on the fly

```
W_h = torch.randn(20, 20, requires_grad=True)
W_x = torch.randn(20, 10, requires_grad=True)
x = torch.randn(1, 10)
prev_h = torch.randn(1, 20)
```

Training

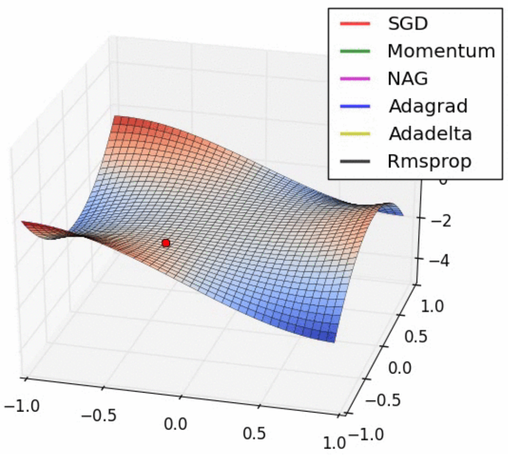


Sample labeled data (**batch**)

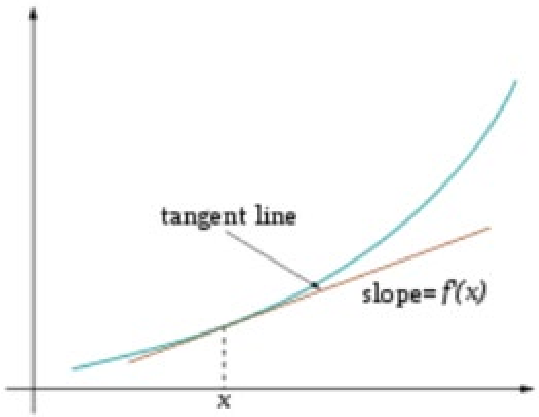
Forward it through the network, get predictions

Back-propagate the errors

Update the network weights



Optimize (min. or max.) **objective/cost function $J(\theta)$**
Generate **error signal** that measures difference between predictions and target values



Use error signal to change the **weights** and get more accurate predictions
Subtracting a fraction of the **gradient** moves you towards the **(local) minimum of the cost function**

https://medium.com/@ramrajchandradevan/the-evolution-of-gradient-descend-optimization-algorithm-4106a6702d39

Acknowledgement

- Part A used materials from: Christopher Bishop, Neil Lawrence, Lee Harrison, John Gosling, Chuck Huber

- Part B used materials from: Ismini Lourentzou, Fei-Fei Li & Justin Johnson & Serena Yeung, Rui Zhang, Nelson Liu

Recommended Reading

- PRML book: Section 3.3 on Bayesian Linear Regression
- The lab notebook and references there