

Lecture 1 and 2: Probabilistic Regression

Machine Learning 4F13, Spring 2014

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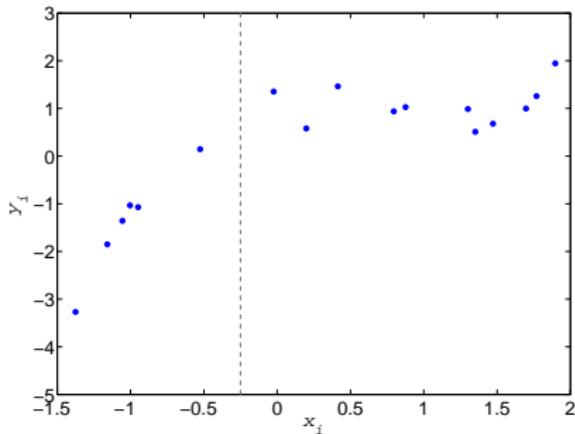
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Key concepts

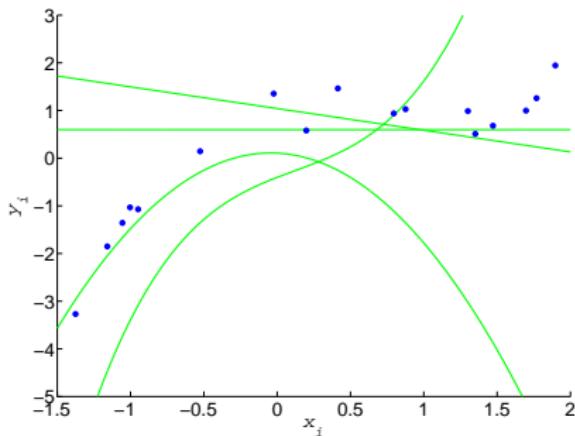
- Linear in the parameters models
 - the concept of a model
 - making predictions
 - least squares fitting
 - limitation: overfitting
- Likelihood and the concept of noise
 - Gaussian iid noise
 - maximum likelihood fitting
 - equivalence to least squares
 - motivation for inference with multiple hypotheses

How do we fit this dataset?



- Dataset $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$ of N pairs of inputs x_i and targets y_i . This data can for example be measurements in an experiment.
- Goal: predict target y_* associated to any arbitrary input x_* . This is known as a **regression** task in machine learning.
- Note: Here the inputs are scalars, we have a single **input feature**. Inputs to regression tasks are often vectors of multiple input features.

Model of the data

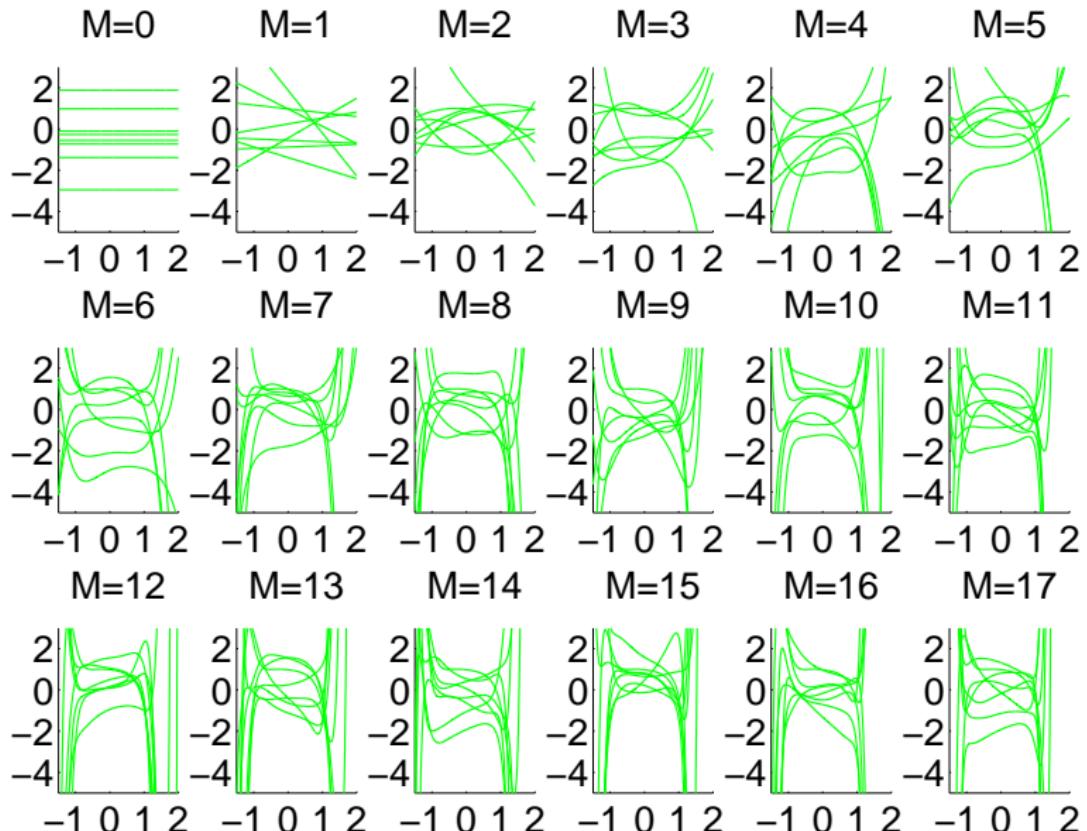


- In order to predict at a new x_* we need to postulate a model of the data. We will estimate y_* with $f(x_*)$.
- But what is $f(x)$? Example: a polynomial

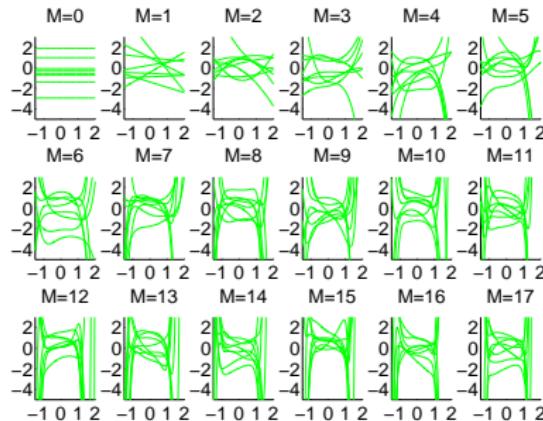
$$f_w(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \dots + w_M x^M$$

The w_j are the weights of the polynomial, the **parameters** of the model.

Model of the data. Example: polynomials of degree M

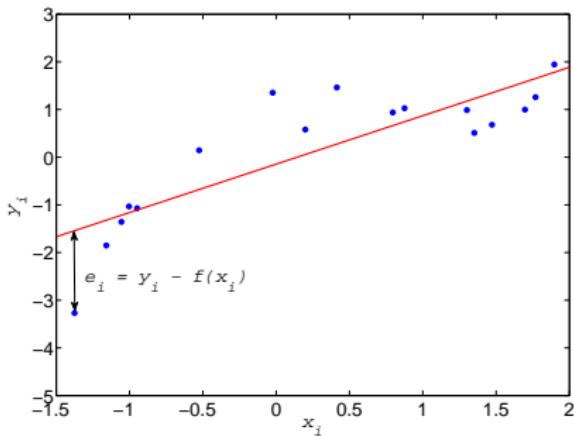


Model structure and model parameters



- Should we choose a polynomial? model structure
- What degree should we choose for the polynomial? model structure
- For a given degree, how do we choose the weights? model parameters
- For now, let's find the single "best" polynomial: degree and weights.

Fitting model parameters: the least squares approach



- Idea: measure the quality of the fit to the training data.
- For each training point, measure the squared error $e_i^2 = (y_i - f(x_i))^2$.
- Find the parameters that minimise the sum of squared errors:

$$E(\mathbf{w}) = \sum_{i=1}^N e_i^2$$

$f_{\mathbf{w}}(x)$ is a function of the parameter vector $\mathbf{w} = [w_0, w_1, \dots, w_M]^T$.

Least squares in detail. (1) Notation

Some notation: training targets y , predictions f and errors e .

- $y = [y_1, \dots, y_N]^\top$ is a vector that stacks the N training targets.
- $f = [f_w(x_1), \dots, f_w(x_N)]^\top$ stacks $f_w(x)$ evaluated at the N training inputs.
- $e = y - f$ is the vector of training prediction errors.

The sum of squared errors is therefore given by

$$E(w) = \|e\|^2 = e^\top e = (y - f)^\top (y - f)$$

More notation: weights w , basis functions $\phi_j(x)$ and matrix Φ .

- $w = [w_0, w_1, \dots, w_M]^\top$ stacks the $M + 1$ model weights.
- $\phi_j(x) = x^j$ is a **basis function** of our **linear in the parameters** model.

$$f_w(x) = w_0 \textcolor{red}{1} + \textcolor{blue}{w_1} x + \textcolor{red}{w_2} x^2 + \dots + \textcolor{blue}{w_M} x^M = \sum_{j=0}^M \textcolor{blue}{w_j} \phi_j(x)$$

- $\Phi_{ij} = \phi_j(x_i)$ allows us to write $f = \Phi w$.

Least squares in detail. (2) Solution

A Gradient View. The sum of squared errors is a convex function of \mathbf{w} :

$$E(\mathbf{w}) = (\mathbf{y} - \mathbf{f})^\top (\mathbf{y} - \mathbf{f}) = (\mathbf{y} - \Phi \mathbf{w})^\top (\mathbf{y} - \Phi \mathbf{w})$$

The gradient with respect to the weights is:

$$\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = -2 \Phi^\top (\mathbf{y} - \Phi \mathbf{w}) = -2 \Phi^\top \mathbf{y} + 2 \Phi^\top \Phi \mathbf{w}$$

The weight vector $\hat{\mathbf{w}}$ that sets the gradient to zero minimises $E(\mathbf{w})$:

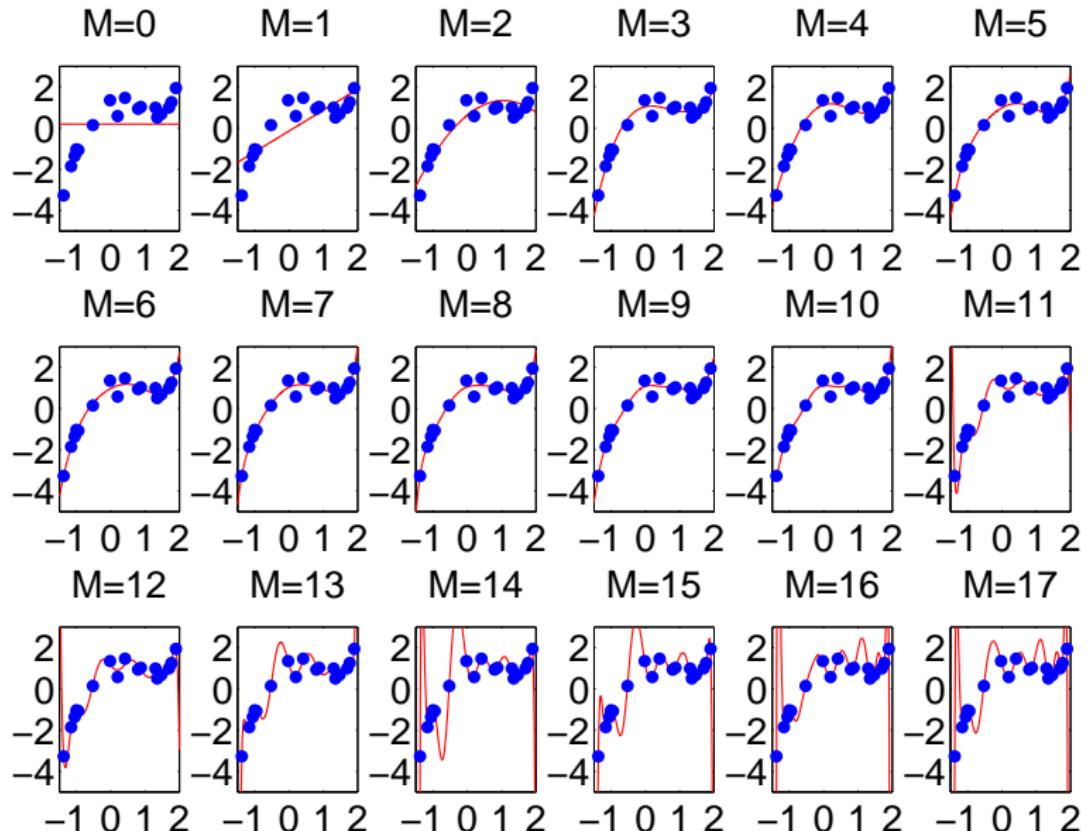
$$\hat{\mathbf{w}} = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{y}$$

A Geometrical View. This is the matrix form of the [Normal equations](#).

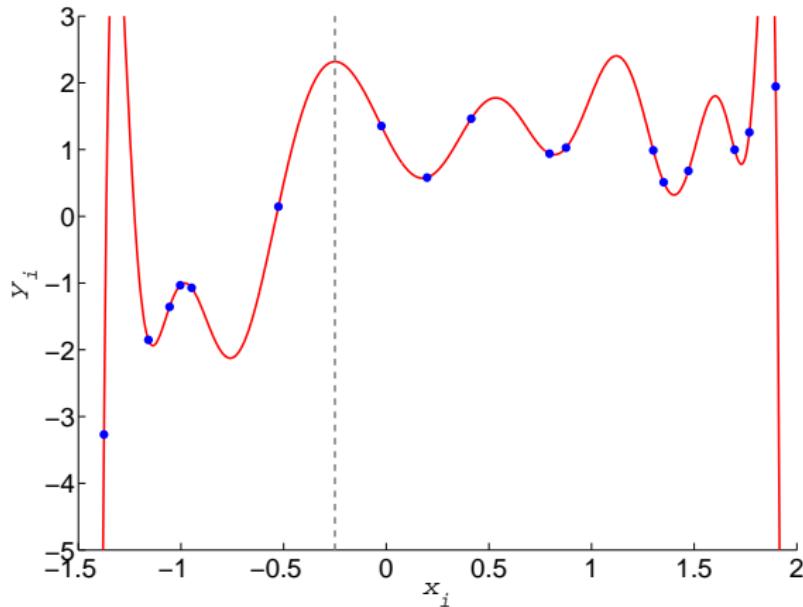
- The vector of training targets \mathbf{y} lives in an N -dimensional vector space.
- The vector of training predictions \mathbf{f} lives in the same space, but it is constrained to being generated by the $M + 1$ columns of matrix Φ .
- The error vector \mathbf{e} is minimal if it is orthogonal to all columns of Φ :

$$\Phi^\top \mathbf{e} = 0 \iff \Phi^\top (\mathbf{y} - \Phi \mathbf{w}) = 0$$

Least squares fit for polynomials of degree 0 to 17

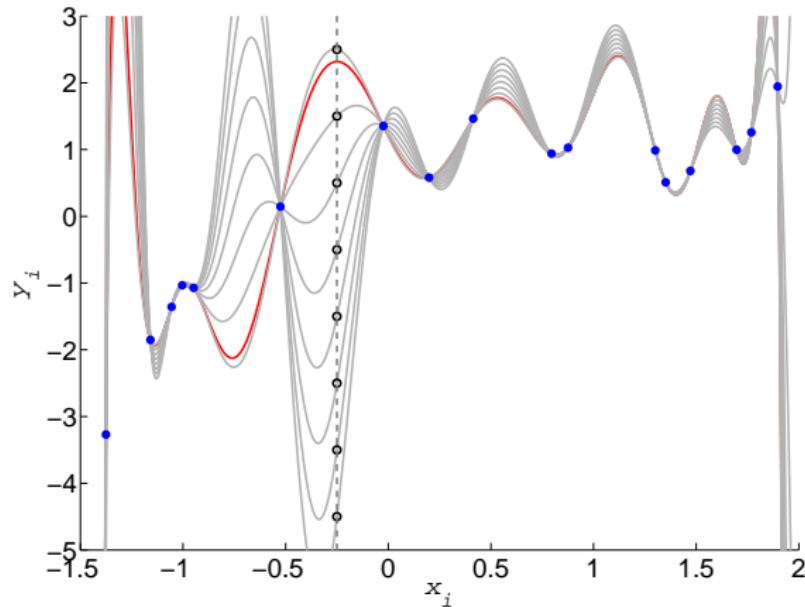


Have we solved the problem?



- Ok, so have we solved the problem?
- What do we think y_* is for $x_* = -0.25$? And for $x_* = 2$?
- If M is large enough, we can find a model that fits the data

Overfitting

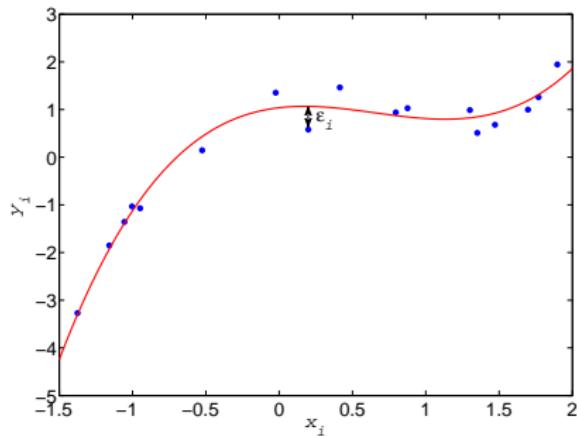


- All the models in the figure are polynomials of degree 17 (18 weights).
- All perfectly fit the 17 training points, plus any desired y_* at $x_* = -0.25$.
- We have not solved the problem. Key missing ingredient: **assumptions!**

A laundry list of open questions

- Do we think that all models are equally probable... **before** we see any data?
What does the probability of a model even mean?
- Do we need to choose a single “best” model or can we consider several?
We need a “language” to represent them.
- Perhaps our training targets are contaminated with noise. What to do?
This question is a bit easier, we will start here.

Observation noise



- Imagine the data was in reality **generated** by the **red function**.
- But each $f(x_*)$ was independently contaminated by a noise term ϵ_i .
- The observations are noisy: $y_i = f_w(x_i) + \epsilon_i$.
- We can characterise the noise with a probability density function.
For example a Gaussian density function, $\epsilon_i \sim \mathcal{N}(\epsilon_i; 0, \sigma_{\text{noise}}^2)$:

$$p(\epsilon_i) = \frac{1}{\sqrt{2\pi\sigma_{\text{noise}}^2}} \exp\left(-\frac{\epsilon_i^2}{2\sigma_{\text{noise}}^2}\right)$$

Probability of the observed data given the model

A vector and matrix notation view of the noise.

- $\epsilon = [\epsilon_1, \dots, \epsilon_N]^\top$ stacks the **independent** noise terms:

$$\epsilon \sim \mathcal{N}(\epsilon; 0, \sigma_{\text{noise}}^2 \mathbf{I}) \quad p(\epsilon) = \prod_{i=1}^N p(\epsilon_i) = \left(\frac{1}{\sqrt{2\pi \sigma_{\text{noise}}^2}} \right)^N \exp \left(-\frac{\epsilon^\top \epsilon}{2 \sigma_{\text{noise}}^2} \right)$$

- Given that $\mathbf{y} = \mathbf{f} + \epsilon$ we can write the probability of \mathbf{y} given \mathbf{f} :

$$\begin{aligned} p(\mathbf{y}|\mathbf{f}, \sigma_{\text{noise}}^2) &= \mathcal{N}(\mathbf{y}; \mathbf{f}, \sigma_{\text{noise}}^2) = \left(\frac{1}{\sqrt{2\pi \sigma_{\text{noise}}^2}} \right)^N \exp \left(-\frac{\|\mathbf{y} - \mathbf{f}\|^2}{2 \sigma_{\text{noise}}^2} \right) \\ &= \left(\frac{1}{\sqrt{2\pi \sigma_{\text{noise}}^2}} \right)^N \exp \left(-\frac{E(\mathbf{w})}{2 \sigma_{\text{noise}}^2} \right) \end{aligned}$$

- $E(\mathbf{w}) = \sum_{i=1}^N (y_i - f_{\mathbf{w}}(x_i))^2 = \|\mathbf{y} - \Phi \mathbf{w}\|^2$ is the sum of squared errors.
- Since $\mathbf{f} = \Phi \mathbf{w}$ we can write $p(\mathbf{y}|\mathbf{w}, \sigma_{\text{noise}}^2) = p(\mathbf{y}|\mathbf{f}, \sigma_{\text{noise}}^2)$ for a given Φ .

Likelihood function

Likelihood of the weights and probability of the data.

- $p(y|w, \sigma_{\text{noise}}^2)$ is the probability of the observed data given the weights.
- $\mathcal{L}(w) \propto p(y|w, \sigma_{\text{noise}}^2)$ is the **likelihood** of the weights given the observed data.

Maximum likelihood.

- We can fit the model weights to the data by maximising the likelihood:

$$\hat{w} = \operatorname{argmax} \mathcal{L}(w) = \operatorname{argmax} \exp\left(-\frac{E(w)}{2\sigma_{\text{noise}}^2}\right) = \operatorname{argmin} E(w)$$

- With an additive Gaussian independent noise model, the **maximum likelihood** and the **least squares** solutions are the same.
- So ... we still have not solved the prediction problem! We still overfit.

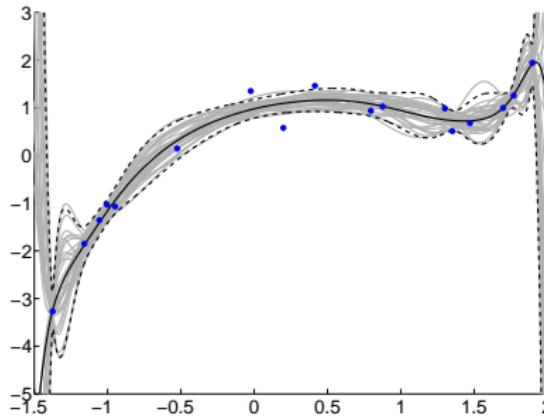
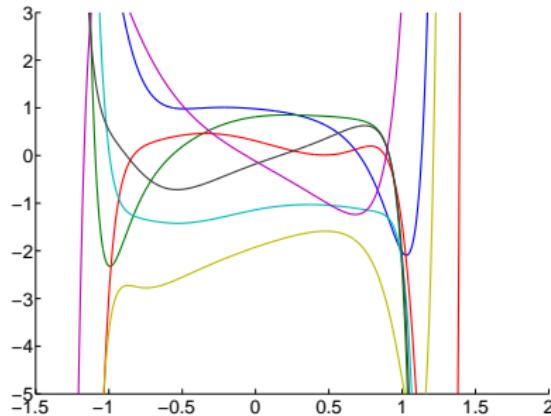
Multiple explanations of the data

Multiple explanations:

- We do not **believe** all models are equally probable to explain the data.
- We may **believe** a simpler model is more probable than a complex one.

Model complexity:

- We do not **know** what particular function generated the data.
- More than one of our models can perfectly fit the data.
- We **believe** more than one of our models could have generated the data.
- We want to reason in terms of **a set of possible explanations**, not just one.



Key Concepts

- probability basics
 - Example: Medical diagnosis
 - joint, conditional and marginal probabilities
 - the two rules of probability: sum and product rules
 - Bayes rule
- Bayesian inference and prediction with finite regression models
 - likelihood and prior
 - posterior and predictive distribution
- the marginal likelihood
 - Bayesian model selection
 - Example: How Bayes avoids overfitting

Medical inference (diagnosis)

Breast cancer facts:

- 1% of scanned women have breast cancer
- 80% of women with breast cancer get positive mammography scans
- 9.6% of women without breast cancer also get positive mammography scans

Question: A woman gets a scan, and it is positive; what is the probability that she has breast cancer?

- ① less than 1%
- ② around 10%
- ③ around 90%
- ④ more than 99%

Medical inference, numerical

Define: C = presence of breast cancer, \bar{C} = no cancer

The probability of cancer for scanned women is $p(C) = 1\%$

If there is cancer, the probability of a positive mammography is $p(M|C) = 80\%$

If there is no cancer, we still have $p(M|\bar{C}) = 9.6\%$

The question is what is $p(C|M)$?

Consider 10000 subjects of screening

- $p(C) = 1\%$, therefore 100 of them have cancer, of which
 - $p(M|C) = 80\%$, therefore 80 get a positive mammography
 - 20 get a negative mammography
- $p(\bar{C}) = 99\%$, therefore 9900 of them do not have cancer, of which
 - $p(M|\bar{C}) = 9.6\%$, therefore 950 get a positive mammography
 - 8950 get a negative mammography

	M	\bar{M}
C	80	20
\bar{C}	950	8950

$p(C|M)$ is obtained as the proportion of all positive mammographies for which there actually is breast cancer

$$p(C|M) = \frac{p(C, M)}{p(C, M) + p(\bar{C}, M)} = \frac{p(C, M)}{p(M)} = \frac{80}{80 + 950} \simeq 7.8\%$$

This is an example of Bayes' rule:

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)}.$$

Which is just a consequence of the definition of *conditional probability*

$$p(A|B) = \frac{p(A, B)}{p(B)}, \quad (\text{where } p(B) \neq 0).$$

Just two rules of probability theory

Astonishingly, the rich theory of probability can be derived using just two rules:

The *sum rule* states that

$$p(A) = \sum_B p(A, B), \quad \text{or} \quad p(A) = \int_B p(A, B) dB,$$

for discrete and continuous variables. Sometimes called *marginalization*.

The *product rule* states that

$$p(A, B) = p(A|B)p(B).$$

It follows directly from the definition of *conditional probability*, and leads directly to *Bayes' rule*

$$p(A|B)p(B) = p(A, B) = p(B|A)p(A) \Rightarrow p(A|B) = \frac{p(B|A)p(A)}{p(B)}.$$

Special case:

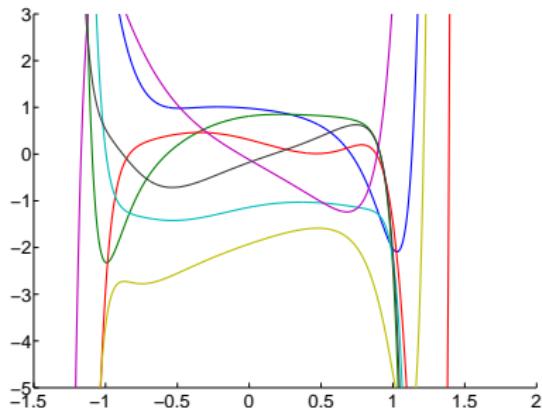
if A and B are *independent*, $p(A|B) = p(A)$, and thus $p(A, B) = p(A)p(B)$.

Posterior probability of a function

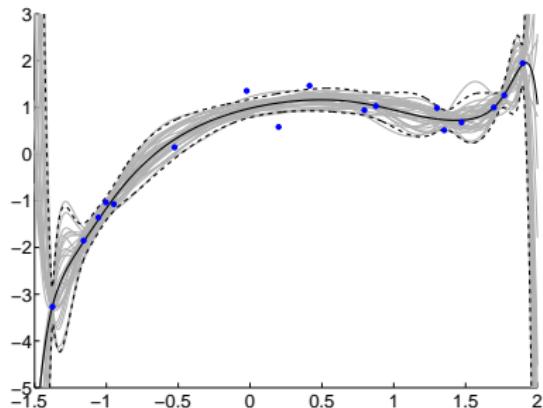
Given the **prior** functions $p(f)$ how can we make predictions?

- Of all functions generated from the prior, keep those that fit the data.
- The notion of closeness to the data is given by the **likelihood** $p(y|f)$.
- We are really interested in the posterior distribution over functions:

$$p(f|y) = \frac{p(y|f) p(f)}{p(y)} \quad \text{Bayes Rule}$$



Some samples from the prior



Samples from the posterior

Priors on parameters induce priors on functions

A model \mathcal{M} is the choice of a **model structure** and of **parameter values**.

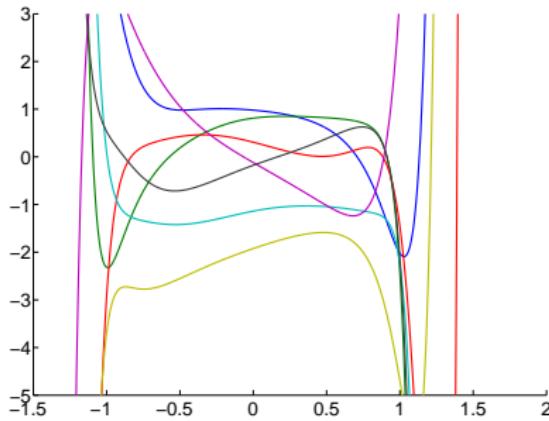
$$f_w(x) = \sum_{j=0}^M w_j \phi_j(x)$$

The prior $p(w|\mathcal{M})$ determines what **functions** this model can generate. Example:

- Imagine we choose $M = 17$, and $p(w_i) = \mathcal{N}(w_i; 0, \sigma_w^2)$.
- We have actually defined a **prior distribution over functions** $p(f|\mathcal{M})$.

This figure is generated as follows:

- Use polynomial basis functions, $\phi_j(x) = x^j$.
- Define a uniform grid of $n = 100$ values in $x [-1.5, 2]$.
- Generate matrix Φ for $M = 17$.
- Draw $w_i \sim \mathcal{N}(0, 1)$.
- Compute and plot $f = \Phi_{n \times 18} w$.



Maximum likelihood, parametric model

Supervised parametric learning:

- data: \mathbf{x}, \mathbf{y}
- model \mathcal{M} : $y = f_{\mathbf{w}}(\mathbf{x}) + \varepsilon$

Gaussian likelihood:

$$p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M}) \propto \prod_{i=1}^N \exp\left(-\frac{1}{2}(y_i - f_{\mathbf{w}}(x_i))^2 / \sigma_{\text{noise}}^2\right).$$

Maximize the likelihood:

$$\mathbf{w}_{\text{ML}} = \underset{\mathbf{w}}{\operatorname{argmax}} p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M}).$$

Make predictions, by plugging in the ML estimate:

$$p(y_*|x_*, \mathbf{w}_{\text{ML}}, \mathcal{M})$$

Bayesian Inference, parametric model

Supervised parametric learning:

- data: \mathbf{x}, \mathbf{y}
- model \mathcal{M} : $y = f_{\mathbf{w}}(\mathbf{x}) + \varepsilon$

Gaussian likelihood:

$$p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M}) \propto \prod_{i=1}^N \exp\left(-\frac{1}{2}(y_i - f_{\mathbf{w}}(x_i))^2 / \sigma_{\text{noise}}^2\right).$$

Parameter prior:

$$p(\mathbf{w}|\mathcal{M})$$

Posterior parameter distribution by Bayes rule $p(a|b) = p(b|a)p(a)/p(b)$:

$$p(\mathbf{w}|\mathbf{x}, \mathbf{y}, \mathcal{M}) = \frac{p(\mathbf{w}|\mathcal{M})p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M})}{p(\mathbf{y}|\mathbf{x}, \mathcal{M})}$$

Bayesian inference, parametric model, cont.

Posterior parameter distribution by Bayes rule $p(a|b) = p(b|a)p(a)/p(b)$:

$$p(w|x, y, \mathcal{M}) = \frac{p(w|\mathcal{M})p(y|x, w, \mathcal{M})}{p(y|x, \mathcal{M})}$$

Making predictions (marginalizing out the parameters):

$$\begin{aligned} p(y_*|x_*, x, y, \mathcal{M}) &= \int p(y_*, w|x, y, x_*, \mathcal{M}) dw \\ &= \int p(y_*|w, x_*, \mathcal{M})p(w|x, y, \mathcal{M}) dw. \end{aligned}$$

Posterior and predictive distribution in detail

For a linear in the parameters model with Gaussian priors and Gaussian noise:

- Gaussian *prior* on the weights: $p(\mathbf{w}|\mathcal{M}) = \mathcal{N}(\mathbf{w}; \mathbf{0}, \sigma_w^2 \mathbf{I})$
- Gaussian *likelihood* of the weights: $p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M}) = \mathcal{N}(\mathbf{y}; \Phi \mathbf{w}, \sigma_{\text{noise}}^2 \mathbf{I})$

Posterior parameter distribution by Bayes rule $p(a|b) = p(b|a)p(a)/p(b)$:

$$p(\mathbf{w}|\mathbf{x}, \mathbf{y}, \mathcal{M}) = \frac{p(\mathbf{w}|\mathcal{M})p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M})}{p(\mathbf{y}|\mathbf{x}, \mathcal{M})} = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$\boldsymbol{\Sigma} = \left(\sigma_{\text{noise}}^{-2} \Phi^\top \Phi + \sigma_w^{-2} \mathbf{I} \right)^{-1} \quad \text{and} \quad \boldsymbol{\mu} = \left(\Phi^\top \Phi + \frac{\sigma_{\text{noise}}^2}{\sigma_w^2} \mathbf{I} \right)^{-1} \Phi^\top \mathbf{y}$$

The predictive distribution is given by:

$$p(\mathbf{y}_*|\mathbf{x}_*, \mathbf{x}, \mathbf{y}, \mathcal{M}) = \mathcal{N}(\mathbf{y}_*; \Phi(\mathbf{x}_*)^\top \boldsymbol{\mu}, \Phi(\mathbf{x}_*)^\top \boldsymbol{\Sigma} \Phi(\mathbf{x}_*) + \sigma_{\text{noise}}^2)$$

Marginal likelihood

$$p(\mathbf{w}|\mathbf{x}, \mathbf{y}, \mathcal{M}) = \frac{p(\mathbf{w}|\mathcal{M})p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M})}{p(\mathbf{y}|\mathbf{x}, \mathcal{M})}$$

Marginal likelihood:

$$p(\mathbf{y}|\mathbf{x}, \mathcal{M}) = \int p(\mathbf{w}|\mathcal{M})p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M})d\mathbf{w}.$$

Second level inference: model comparison and Bayes' rule again

$$p(\mathcal{M}|\mathbf{y}, \mathbf{x}) = \frac{p(\mathbf{y}|\mathbf{x}, \mathcal{M})p(\mathcal{M})}{p(\mathbf{y}|\mathbf{x})} \propto p(\mathbf{y}|\mathbf{x}, \mathcal{M})p(\mathcal{M}).$$

The *marginal likelihood* is used to select between models.

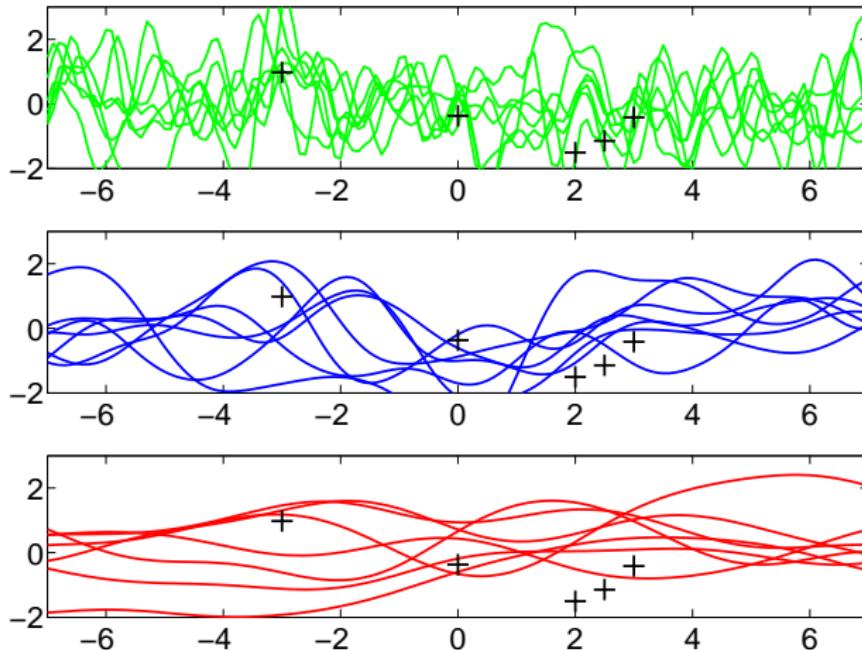
For linear in the parameter models with Gaussian priors and noise:

$$p(\mathbf{y}|\mathbf{x}, \mathcal{M}) = \int p(\mathbf{w}|\mathcal{M})p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \mathcal{M})d\mathbf{w} = \mathcal{N}(\mathbf{y}; \mathbf{0}, \sigma_w^2 \boldsymbol{\Phi} \boldsymbol{\Phi}^\top + \sigma_{\text{noise}}^2 \mathbf{I})$$

Understanding the marginal likelihood (1). Models

Consider 3 models \mathcal{M}_1 , \mathcal{M}_2 and \mathcal{M}_3 . Given our data:

- We want to compute the *marginal likelihood* for each model.
- We want to obtain the predictive distribution for each model.



Understanding the marginal likelihood (2). Noise

Consider a very simple noise model for $y_i = f(x_i) + \epsilon_i$

- $\epsilon_i \sim \text{Uniform}(-0.2, 0.2)$ and all noise terms are independent.
- $p(y_i|f(x_i)) = 0$ if $|y_i - f(x_i)| > 0.2$, and $p(y_i|f(x_i)) = 1/0.4 = 2.5$ otherwise.
- The likelihood of a given function from the prior is

$$p(y|f) = \prod_{i=1}^N p(y_i|f(x_i)) = \begin{cases} 0 & \text{if for any } i, |y_i - f(x_i)| > 0.2 \\ 2.5^N & \text{otherwise} \end{cases}$$

We will approximate the marginal likelihood by *Monte Carlo*:

$$p(y|\mathcal{M}_i) = \int p(y|f) p(f|\mathcal{M}_i) df \approx \frac{1}{S} \sum_{s=1}^S p(y|f_s) = \frac{S_a}{S} \cdot 2.5^N$$

- A total of S functions are sampled from the prior $p(f|\mathcal{M}_i)$.
- f_s is the s^{th} function sampled from the prior.
- S_a is the number of samples with non-zero likelihood: these are accepted. The remaining $S - S_a$ samples are rejected.

Simple Monte Carlo

We can approximate integrals of the form

$$z = \int f(x)p(x)dx,$$

where $p(x)$ is a probability distribution, using a sum

$$z \simeq \frac{1}{T} \sum_{t=1}^T f(x^{(t)}), \text{ where } x^{(t)} \sim p(x).$$

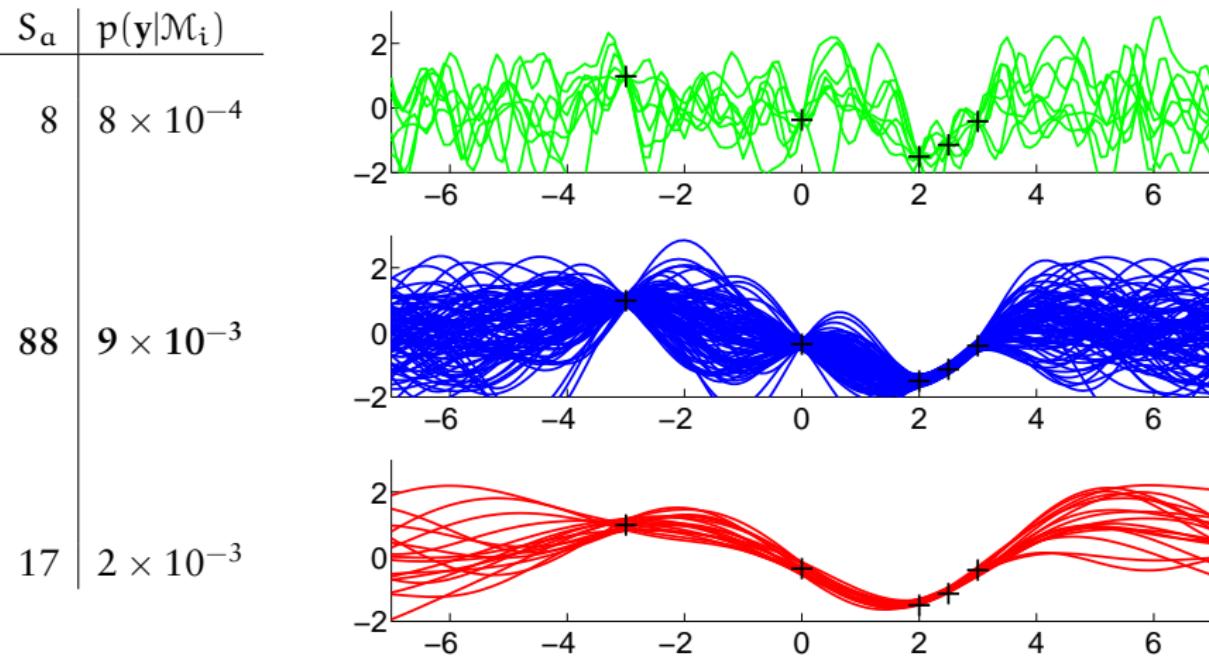
As $T \rightarrow \infty$ the approximation (under very mild conditions) converges to z .

This algorithm is called *Simple Monte Carlo*.

Understanding the marginal likelihood (3). Posterior

Posterior samples for each of the models obtained by rejection sampling.

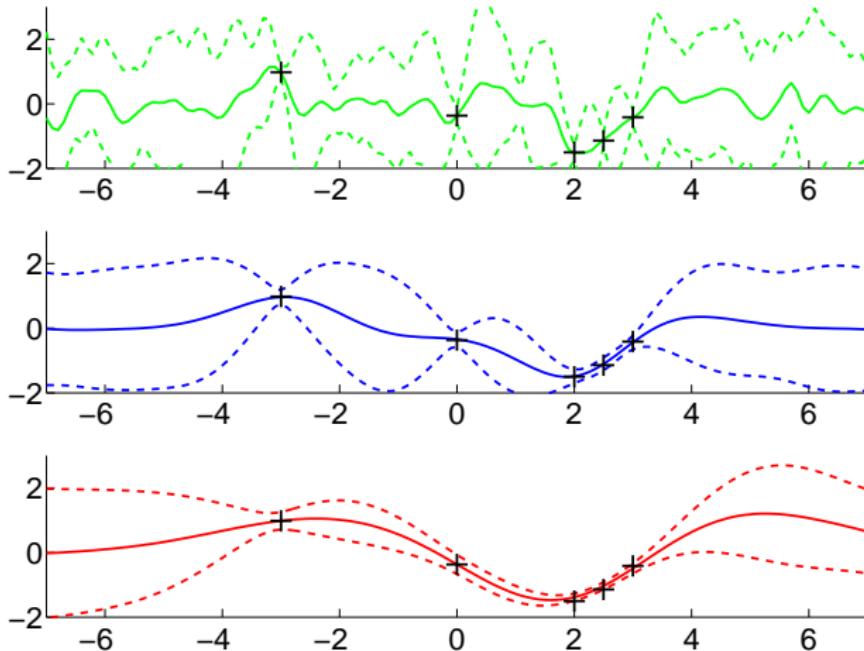
- For each model we draw 1 million samples from the prior.
- We only keep the samples that have non-zero likelihood.



Predictive distribution

Predictive distribution for each of the models obtained.

- For each model we take all the posterior functions from rejection sampling.
- We compute the average and standard deviation of $f_s(x_i)$.



Conclusions

Probability theory provides a framework for

- making inferences from data in a model
- making probabilistic predictions

It also provides a *principled* and *automatic* way of doing

- model comparison

In the following lectures, we'll demonstrate how to use this framework to solve challenging machine learning problems.

Appendix: Some useful Gaussian identities

If \mathbf{x} is multivariate Gaussian with mean μ and covariance matrix Σ

$$p(\mathbf{x}; \mu, \Sigma) = (2\pi|\Sigma|)^{-D/2} \exp\left(-(\mathbf{x} - \mu)^\top \Sigma^{-1}(\mathbf{x} - \mu)/2\right),$$

then

$$\mathbb{E}[\mathbf{x}] = \mu,$$

$$\mathbb{V}[\mathbf{x}] = \mathbb{E}[(\mathbf{x} - \mathbb{E}[\mathbf{x}])^2] = \Sigma.$$

For any matrix A , if $\mathbf{z} = A\mathbf{x}$ then \mathbf{z} is Gaussian and

$$\mathbb{E}[\mathbf{z}] = A\mu,$$

$$\mathbb{V}[\mathbf{z}] = A\Sigma A^\top.$$