Probabilistic Machine Learning
Lecture 07
Parametric Regression

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Recap: Gaussian Distributions

Gaussian distributions provide the linear algebra of inference

- products of Gaussians are Gaussians $\qquad C := (A^{-1} + B^{-1})^{-1} \quad c := C(A^{-1}a + B^{-1}b)$

$$\mathcal{N}(x; a, A)\mathcal{N}(x; b, B) = \mathcal{N}(x; c, C)\mathcal{N}(a; b, A + B)$$

- linear projections of Gaussians are Gaussians

$$p(z) = \mathcal{N}(z; \mu, \Sigma) \quad \Rightarrow \quad p(Az) = \mathcal{N}(Az, A\mu, A\Sigma A^\intercal)$$

- marginals of Gaussians are Gaussians

$$\int \mathcal{N}\left[\begin{bmatrix} x \\ y \end{bmatrix}; \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}, \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix}\right] dy = \mathcal{N}(x; \mu_x, \Sigma_{xx})$$

- (linear) conditionals of Gaussians are Gaussians

$$p(x \mid y) = \frac{p(x, y)}{p(y)} = \mathcal{N}\left(x; \mu_x + \Sigma_{xy}\Sigma_{yy}^{-1}(y - \mu_y), \Sigma_{xx} - \Sigma_{xy}\Sigma_{yy}^{-1}\Sigma_{yx}\right)$$

Bayesian inference becomes linear algebra $\qquad p(x) = \mathcal{N}(x; \mu, \Sigma) \qquad p(y \mid x) = \mathcal{N}(y; A^\intercal x + b, \Lambda)$

$$p(B^\intercal x + c \mid y) = \mathcal{N}[B^\intercal x + c; B^\intercal \mu + c + B^\intercal \Sigma A(A^\intercal \Sigma A + \Lambda)^{-1}(y - A^\intercal \mu - b), B^\intercal \Sigma B - B^\intercal \Sigma A(A^\intercal \Sigma A + \Lambda)^{-1}A^\intercal \Sigma B]$$

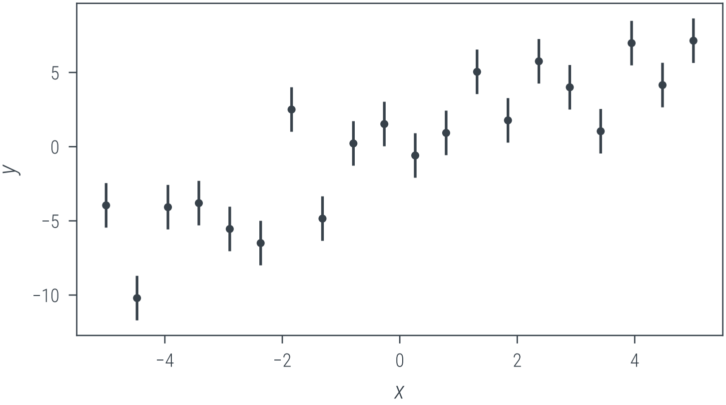
Code

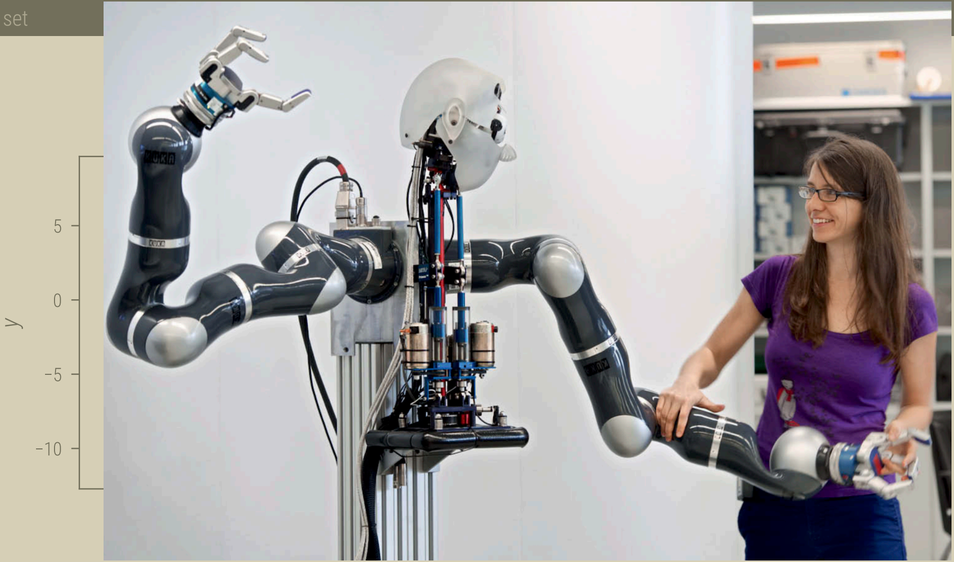
`gaussians.py`

Supervised Regression

A data set

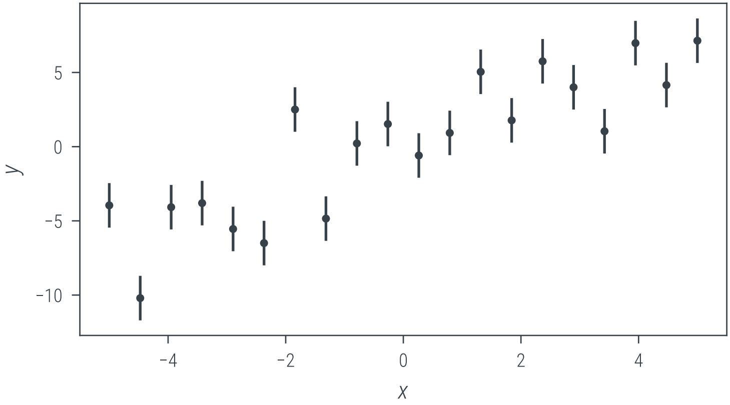
given: $\boldsymbol{y} \in \mathbb{R}^N, \quad p(\boldsymbol{y} \mid f) = \mathcal{N}(\boldsymbol{y}; \boldsymbol{f}(\boldsymbol{x}), \sigma^2 I_N).$ What is f?



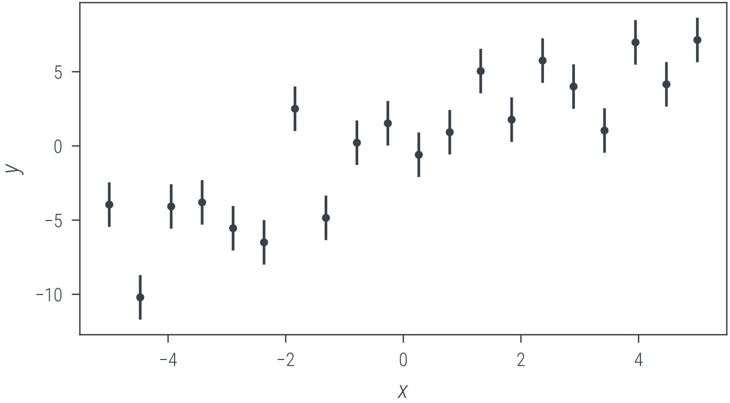

5
0
−5
−10
y

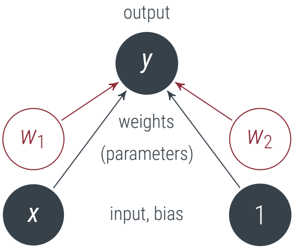
A data set

given: $\boldsymbol{y} \in \mathbb{R}^N, \quad p(\boldsymbol{y} \mid f) = \mathcal{N}(\boldsymbol{y}; \boldsymbol{f}(\boldsymbol{x}), \sigma^2 I_N).$ What is f?



Assume **linear** function $f(x) = w_1 + w_2 x = \phi_x^\intercal \mathbf{w}$ with **features** $\phi(x) = \begin{bmatrix} 1 \\ x \end{bmatrix} =: \phi_x$

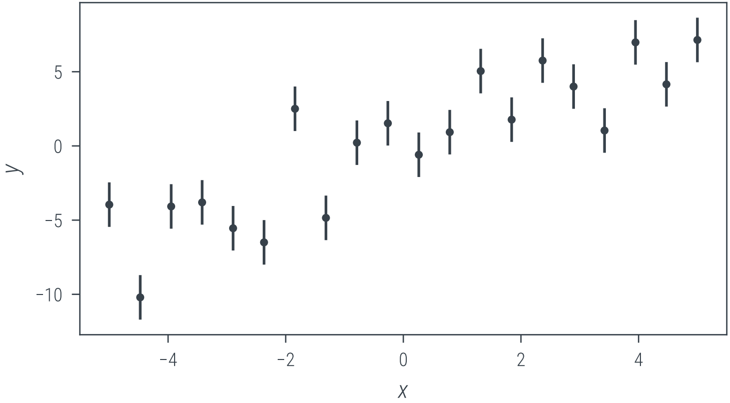


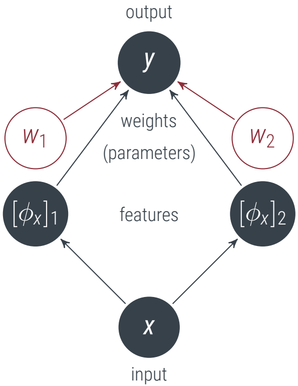


A Linear Model

linear regression

Assume **linear** function $f(x) = w_1 + w_2 x = \phi_x^\intercal w$ with **features** $\phi(x) = \begin{bmatrix} 1 \\ x \end{bmatrix} =: \phi_x$



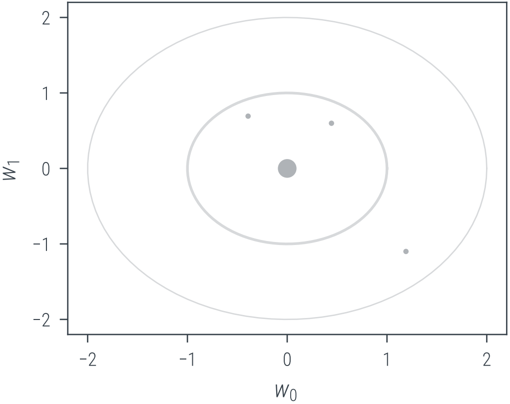


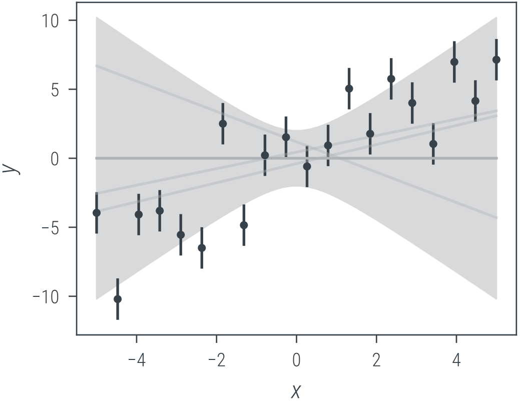
A linear **generative** model

if every variable is Gaussian and every relationship is linear, all marginals and conditionals are also Gaussian

$$f(x) = w_1 + w_2 x = \phi_x^\intercal w$$
$$p(w) = \mathcal{N}(w; \mu, \Sigma)$$

$$p(f) = \mathcal{N}(f; \phi_x^\intercal \mu, \phi_x^\intercal \Sigma \phi_x)$$





Notation

this will become exceedingly helpful later on

Dataset: $X := \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{X}^N, \boldsymbol{y} := \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N$. We will use the following very sloppy notation, sloppily

$$\phi_x := \phi(x) = \begin{bmatrix} 1 \\ x \end{bmatrix} \in \mathbb{R}^F \qquad \phi_X := \begin{bmatrix} \phi(x_1) & \phi(x_2) & \cdots & \phi(x_N) \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_N \end{bmatrix} \in \mathbb{R}^{F \times N}$$

$$f_x := f(x) \in \mathbb{R} \qquad f_X := \phi_X^\intercal \boldsymbol{w} = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) \\ \phi_1(x_2) & \phi_2(x_2) \\ \vdots & \vdots \\ \phi_1(x_N) & \phi_2(x_N) \end{bmatrix} \cdot \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} \phi_{x_1}^\intercal \boldsymbol{w} \\ \phi_{x_2}^\intercal \boldsymbol{w} \\ \vdots \\ \phi_{x_N}^\intercal \boldsymbol{w} \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_N) \end{bmatrix} \in \mathbb{R}^N$$

Think of f as an infinitely long vector, indexed by x:

$$\boldsymbol{v} \in \mathbb{R}^N, I \in \mathbb{N}^d \Rightarrow v_I := [v_{I_1}, \dots, v_{I_d}] \in \mathbb{R} \quad \Longleftrightarrow \quad f \in \mathbb{R}^\infty, X \in \mathbb{R}^N \Rightarrow f_X := [f_{x_1}, \dots, f_{x_N}] \in \mathbb{R}^N.$$

Code

our work pays off

```python
from gaussians import Gaussian
from jax import numpy as jnp

# define prior in weight space
prior = Gaussian(mu=jnp.zeros(2), Sigma=jnp.eye(2))
# map into function space
phi = lambda x: jnp.hstack([jnp.ones_like(x), x])
x = jnp.linspace(-5, 5, 100)[:, None]
f_prior = phi(x) @ prior
```

Gaussian Inference on a linear function

weight space / function space

$$\text{prior} \quad p(w) = \mathcal{N}(w; \mu, \Sigma) \quad \Rightarrow \quad p(f) = \mathcal{N}(f_x; \phi_x^\intercal \mu, \phi_x \Sigma \phi_x)$$

$$\text{likelihood} \quad p(y \mid w, \phi_X) = \mathcal{N}(y; \phi_X^\intercal w, \sigma^2 I) = \mathcal{N}(y; f_X, \sigma^2 I)$$

Gaussian Inference on a linear function

weight space / function space

$$
\begin{aligned}
\text{prior} \quad p(w) &= \mathcal{N}(w; \mu, \Sigma) \quad \Rightarrow \quad p(f) = \mathcal{N}(f_x; \phi_X^\intercal \mu, \phi_x \Sigma \phi_x) \\
\text{likelihood} \quad p(y \mid w, \phi_X) &= \mathcal{N}(y; \phi_X^\intercal w, \sigma^2 I) = \mathcal{N}(y; f_X, \sigma^2 I) \\
\text{posterior on } \boldsymbol{w} \quad p(w \mid \boldsymbol{y}, \phi_X) &= \mathcal{N}(w; \mu + \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(\boldsymbol{y} - \phi_X^\intercal \mu), \\
&\qquad \Sigma - \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1} \phi_X^\intercal \Sigma) \\
&= \mathcal{N}\left(w; (\Sigma^{-1} + \sigma^{-2}\phi_X \phi_X^\intercal)^{-1} \left(\Sigma^{-1}\mu + \sigma^{-2}\phi_X \boldsymbol{y}\right),\right. \\
&\qquad \left.(\Sigma^{-1} + \sigma^{-2}\phi_X \phi_X^\intercal)^{-1}\right)
\end{aligned}
$$

Gaussian Inference on a linear function

weight space / function space

$$
\begin{aligned}
\text{prior} \quad p(w) &= \mathcal{N}(w; \mu, \Sigma) \quad \Rightarrow \quad p(f) = \mathcal{N}(f_x; \phi_x^\intercal \mu, \phi_x \Sigma \phi_x) \\
\text{likelihood} \quad p(y \mid w, \phi_X) &= \mathcal{N}(y; \phi_X^\intercal w, \sigma^2 I) = \mathcal{N}(y; f_X, \sigma^2 I) \\
\text{posterior on } \boldsymbol{w} \quad p(w \mid \boldsymbol{y}, \phi_X) &= \mathcal{N}(w; \mu + \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(\boldsymbol{y} - \phi_X^\intercal \mu), \\
&\qquad \Sigma - \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}\phi_X^\intercal \Sigma) \\
&= \mathcal{N}\left(w; (\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\left(\Sigma^{-1}\mu + \sigma^{-2}\phi_X \boldsymbol{y}\right),\right. \\
&\qquad \left.(\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\right) \\
\text{posterior on } f \quad p(f_x \mid y, \phi_X) &= \mathcal{N}(f_x; \phi_x^\intercal \mu + \phi_x^\intercal \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(y - \phi_X^\intercal \mu), \\
&\qquad \phi_x^\intercal \Sigma \phi_x - \phi_x^\intercal \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}\phi_X^\intercal \Sigma \phi_x) \\
&\qquad \mathcal{N}\left(f_x; \phi_x(\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\left(\Sigma^{-1}\mu + \sigma^{-2}\phi_X \boldsymbol{y}\right),\right. \\
&\qquad \left.\phi_x(\Sigma^{-1} + \sigma^{-2}\phi_X\phi_X^\intercal)^{-1}\phi_x^\intercal\right)
\end{aligned}
$$

Code

our work from last lecture pays off

$$p(w \mid y, \phi_X) = \mathcal{N}\left(w; \mu + \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(y - \phi_X^\intercal \mu), \Sigma - \Sigma\phi_X(\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}\phi_X^\intercal \Sigma\right)$$

```python
from gaussians import Gaussian
from jax import numpy as jnp

# define prior in weight space
prior = Gaussian(mu=jnp.zeros(2), Sigma=jnp.eye(2))
# map into function space
phi = lambda x: jnp.hstack([jnp.ones_like(x), x])
x = jnp.linspace(-5, 5, 100)[:, None]
f_prior = phi(x) @ prior

# load data
import scipy.io
lin_data = scipy.io.loadmat("lindata.mat")
X = lin_data["X"]  # inputs
Y = lin_data["Y"][:, 0]  # outputs
sigma = lin_data["sigma"][0].flatten() # noise

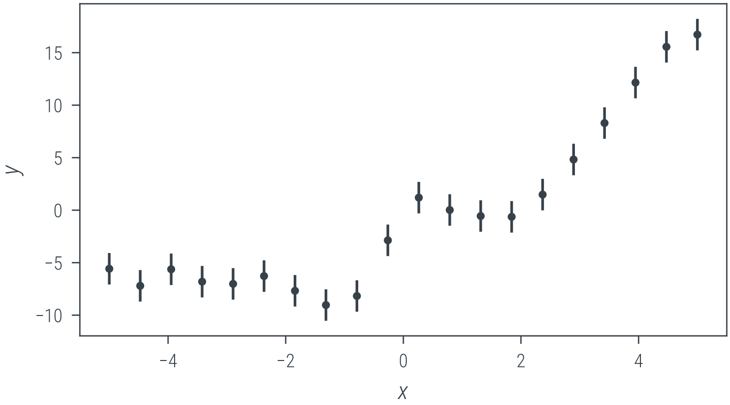
# condition on data to get the posterior: p(w|X,Y) = N(Y|phi(X) @ w, sigma**2 I) * p(w) / p(Y|X)
posterior = prior.condition(phi(X), Y, sigma**2 * jnp.eye(len(X)))
```

DEMO

- `git clone https://github.com/philipphennig/ProbML_Apps.git`
- `cd ProbML_Apps/07`
- `pip install -r requirements.txt`
- `streamlit run Lecture_07.py`

A more Realistic Dataset

General linear regression



$$f(x) = w_1 + w_2 x = \phi_x^\intercal w$$

$$\phi_x := \begin{bmatrix} 1 \\ x \end{bmatrix}$$

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Summary:

- Gaussian distributions can be used to learn functions
- Analytical inference is possible using general linear models

$$f(x) = \phi(x)^\intercal w = \phi_x^\intercal w$$

- Then the posterior on both w and f is Gaussian
- The choice of features $\phi : \mathbb{X} \rightharpoonup \mathbb{R}$ is essentially unconstrained

Please cite this course, as

```
@techreport{Tuebingen_ProbML23 ,
    title =
    {Probabilistic Machine Learning},
    author = {Hennig, Philipp},
    series = {Lecture Notes
        in Machine Learning},
    year = {2023},
    institution = {Tübingen AI Center}}
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