```
import numpy as np
import scipy.stats
import matplotlib.pyplot as plt

from bayesian_stats_course_tools.analyse import plot_data, analyse_data

import warnings
warnings.filterwarnings('ignore')
```

Model checking

$\def\E{\operatorname{E}}$ $\def\Var{\operatorname{Var}}$ $\def\Cov{\operatorname{Cov}}$ $\def\dd{\mathrm{d}}$ $\def\ee{\mathrm{e}}$ $\def\Norm{\mathcal{N}}$ $\def\Uniform{\mathcal{U}}$

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The Bayesian data analysis workflow

1. Model the data generating process probabilistically.
2. Condition the generative process on the observed data.
3. Check that the results fit the observed data and improve the model.
    - Compare different models.

Model checking

A first step to check your model is to plot it against the data.

This can be plotting the best-fit model, but better are the posterior predictive distributions.

If there are obvious issues, such as outliers or misspecified errors, making some plots can already flag these problems.

Our eyes can be easily deceived though. For example, strongly correlated data can have *very* unintuitive behaviour of the best-fitting model.

Chi-square goodness-of-fit

If the data $\vec y$ are Gaussian distributed $$ \vec y\sim \Norm\left(\vec \mu(\vec\theta), \Sigma(\vec\theta)\right) $$ then a traditional test of how well our model fits the data is the chi-square test.

Let us assume we have a set $\vec\theta^*$ of "best" model parameters. For example the MAP or mean of the posterior.

If these are the true parameters that generated the data and the data are Gaussian distributed, then the quantity $$ \chi^2(\vec y, \vec\theta^*) = \left(\vec y - \vec\mu(\vec\theta^*)\right)^T\Sigma(\vec\theta^*)^{-1}\left(\vec y - \vec\mu(\vec\theta^*)\right) $$ is distributed as χ^2_ν.

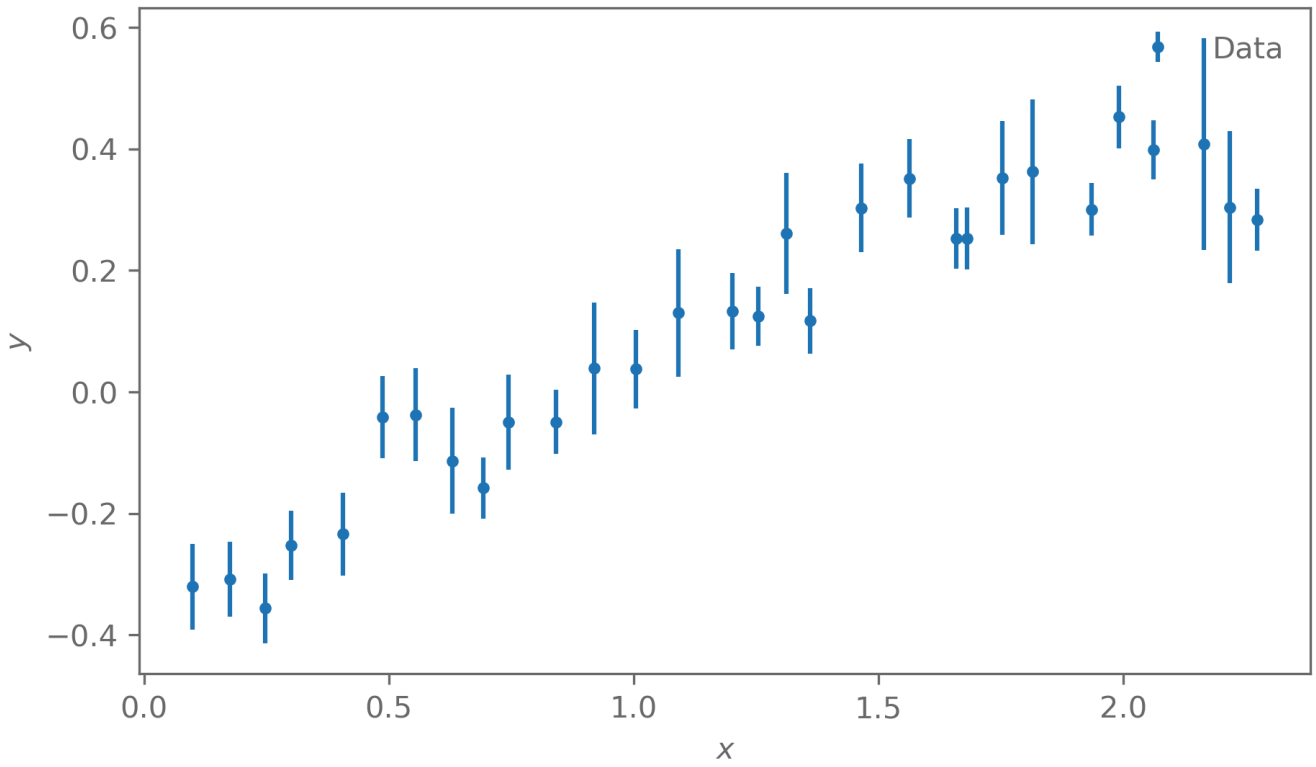
With this we can calculate the probability that the χ^2 statistic would take a higher value in imaginary repeated experiments than the one we have observed $$ \text{Probability to exceed (PTE) } \chi^2(\vec y, \vec\theta^*) = 1 - \mathrm{CDF}\left(\chi^2(\vec y, \vec\theta^*)\right)\ . $$ If the PTE is small, it is unlikely that an experiment would see a χ^2 statistic larger than what we observerd. This indicates that our model is a poor fit to the data.

The number of degrees of freedom is $\nu = n_\mathrm{data} - n_\mathrm{param}$, where n_data is the dimensionality of the data and n_param is the number of constrained parameters.

By fitting the model to the data, we reduce the scatter in the residuals $\vec y - \vec\mu(\theta)$, so the number of degrees of freedom is reduced from n_data by n_param.

Finding n_param in a Bayesian context can be challenging because some parameters might be constrained by the prior, instead of by the likelihood. In this case, they do not reduce the degrees of freedom.

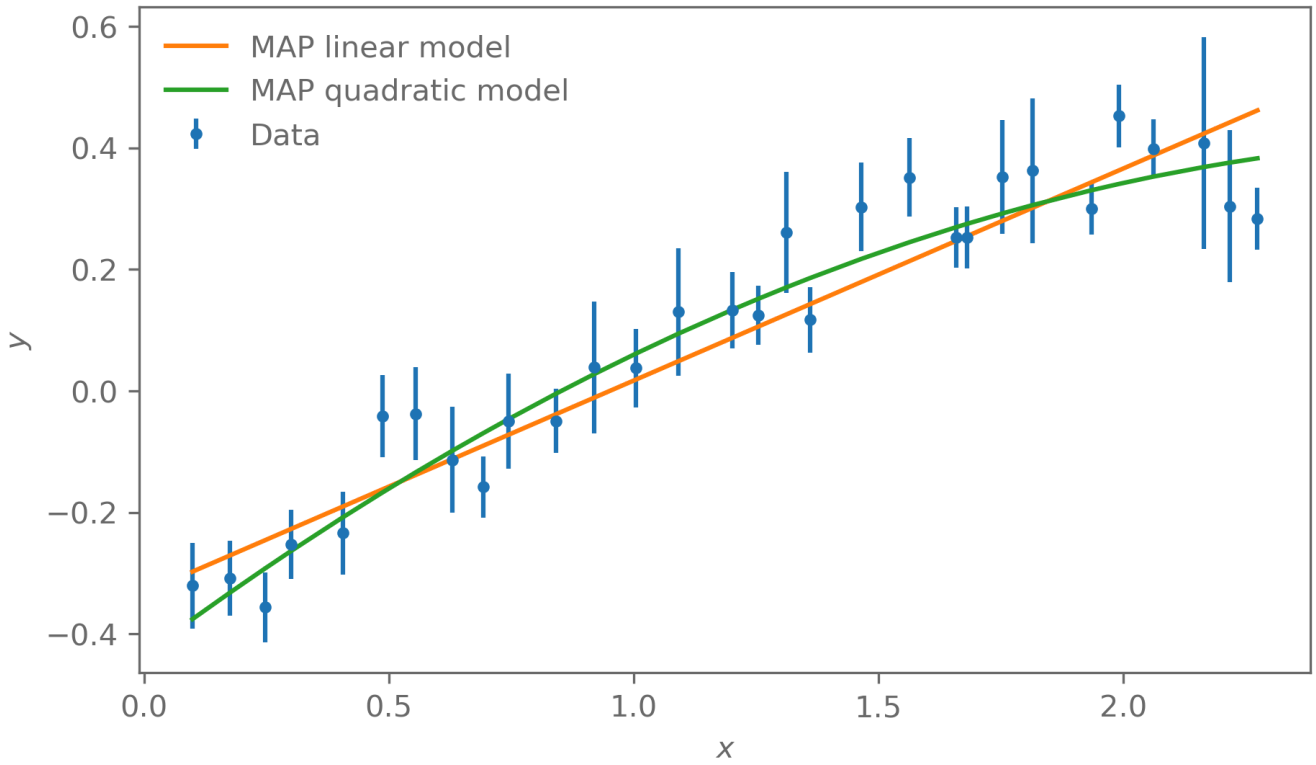
We use the data in `"data/linear_fits/data_2.txt"` has an example and fit both a linear and quadratic model to it.




```
def linear_model(theta, x):
    m, b = theta
    return m*x + b

def log_prior_linear_model(theta):
    m, b = theta
    # Unnormalised uniform prior m\simU(-2, 2), b \sim U(-3, 3)
    if -2 < m < 2 and -3 < b < 3:
        return 0
    else:
        return -np.inf

log_likelihood_lin, log_posterior_lin, predict_lin = \
    make_gaussian_likelihood_components(
        linear_model, log_prior_linear_model
    )
```

```
def quadratic_model(theta, x):
    a, b, c = theta
    return a*x**2 + b*x + c

def log_prior_quadratic_model(theta):
    a, b, c = theta
    # Unnormalised uniform prior m\simU(-2, 2), b \sim U(-3, 3)
    if -1 < a < 1 and -2 < b < 2 and -3 < c < 3:
        return 0
    else:
        return -np.inf

log_likelihood_quad, log_posterior_quad, predict_quad = \
    make_gaussian_likelihood_components(
```

```
        quadratic_model, log_prior_quadratic_model
    )
```



Implement the χ^2 statistic:

```
def chi_squared(y, sigma_y, mu):
    return np.sum((y - mu)**2/sigma_y**2)

chi_squared_linear = chi_squared(
    y, y_err,
    mu=linear_model(results_linear["MAP"], x)
)
chi_squared_quadratic = chi_squared(
    y, y_err,
    mu=quadratic_model(results_quadratic["MAP"], x)
)
```

```
n_data = len(y)
n_param_lin = 2
n_param_quad = 3

PTE_lin = scipy.stats.chi2(df=n_data - n_param_lin).sf(chi_squared_linear)
PTE_quad = scipy.stats.chi2(df=n_data - n_param_quad).sf(chi_squared_quadratic)

print(f"Linear: χ²={chi_squared_linear:.1f}, "
      f"ndof={n_data}-{n_param_lin}, PTE={PTE_lin:.3f}")

print(f"Quadratic: χ²={chi_squared_quadratic:.1f}, "
      f"ndof={n_data}-{n_param_quad}, PTE={PTE_quad:.3f}")
```

```
Linear: χ²=40.8, ndof=30−2, PTE=0.056
Quadratic: χ²=29.3, ndof=30−3, PTE=0.347
```

The quadtratic model fits much better to the data. Note that for the linear model, the probability of getting data that has an even higher χ^2 than we observed is quite low, indicating that the linear model is a poor fit.

Posterior predictive checks

For more details, see chapter 6 in Bayesian Data Analysis

The chi-squared test has two downsides:

- It assumes the data are Gaussian distributed.
- It depends on the effective number of constrained parameters, which can be challenging to define.
- It uses a point estimate for the parameters $\vec\theta^*$ for which to calculate the goodness-of-fit. As Bayesians, we want to avoid point estimates and instead account for the full uncertainty in the posterior.

We use the posterior predictive distribution (PPD) to assess how well our model fits the data.

We define a test statistic $T(y, \theta)$ of the data and the parameters. For example, we could choose the χ^2 statistic $$ T(\vec y, \vec\theta) = \left(\vec y - \vec\mu(\vec\theta)\right)^T\Sigma(\vec\theta)^{-1}\left(\vec y - \vec\mu(\vec\theta)\right) \ . $$

We then sample replicates $\vec y^\mathrm{rep}$ of the data from the PPD $p(\vec y^\mathrm{rep}|\vec y)$. Remember, $$ p(\vec y^\mathrm{rep}|\vec y) = \int p(\vec y^\mathrm{rep}, \vec \theta | \vec y)\dd \theta = \int p(\vec y^\mathrm{rep} |\vec \theta)p(\vec \theta|\vec y)\dd \theta\,. $$

Then compute the probability $$ \Pr\left(T(\vec y^\mathrm{rep}, \vec\theta) \geq T(\vec y, \vec\theta)|\vec y\right)\ . $$

In practice:

1. Sample S samples $\vec\theta_i$ from the posterior $p(\vec\theta|\vec y)$
2. Sample one $\vec y^\mathrm{rep}_i$ from the likelihood $p(\vec y^\mathrm{rep}|\vec\theta_i)$ for each θ_i
3. Count the fraction of samples where $T(\vec y^\mathrm{rep}_i, \vec\theta_i) \geq T(\vec y, \vec\theta_i)$

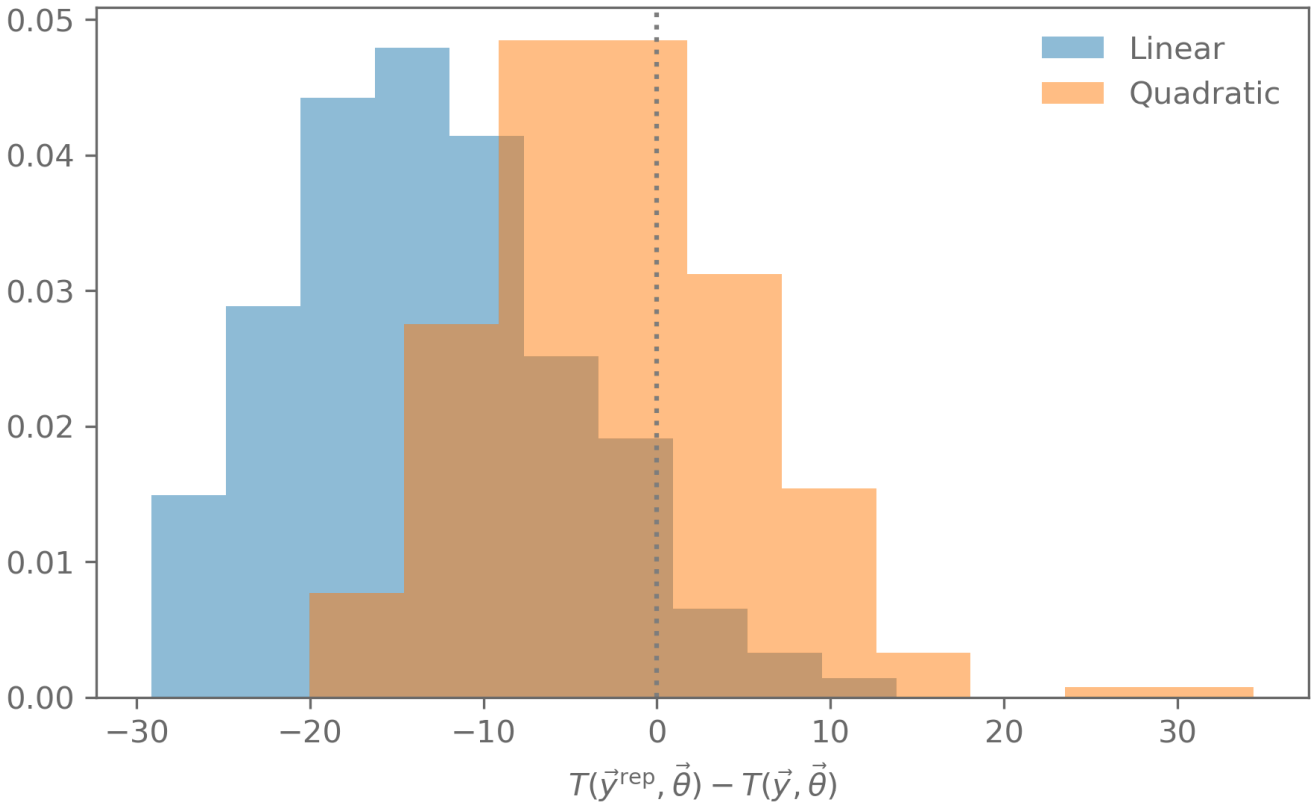
```
def test_statistic(y, theta, x, sigma_y, model):
    mu = model(theta, x)
    t = chi_squared(y, sigma_y, mu)
    return t

def ppd_model_check(test_statistic, y, ppd, ppd_params):
```

```
    t_data = []
    t_rep = []
    for y_rep, theta in zip(ppd, ppd_params):
        t_data.append(test_statistic(y, theta))
        t_rep.append(test_statistic(y_rep, theta))

    t_data = np.array(t_data)
    t_rep = np.array(t_rep)

    pte = (t_rep >= t_data).sum()/len(t_data)
    return pte, t_rep, t_data
```

```
PPD_PTE_lin, t_rep_lin, t_data_lin = ppd_model_check(
    test_statistic=lambda y, theta: test_statistic(
        y, theta, x, y_err, linear_model),
    y=y,
    ppd=results_linear["PPD"],
    ppd_params=results_linear["PPD_params"]
)

PPD_PTE_quad, t_rep_quad, t_data_quad = ppd_model_check(
    test_statistic=lambda y, theta: test_statistic(
        y, theta, x, y_err, quadratic_model),
    y=y,
    ppd=results_quadratic["PPD"],
    ppd_params=results_quadratic["PPD_params"]
)

print(f"Linear: PPD PTE={PPD_PTE_lin:.3f}")
print(f"Quadratic: PPD PTE={PPD_PTE_quad:.3f}")
```

```
Linear: PPD PTE=0.064
Quadratic: PPD PTE=0.372
```

We get quite similar results to the χ^2 test just from samples from the posterior, without further assumptions or point estimates.



Model comparison

After we have checked that the model is describing the data well, we might want to compare different models.

We have already discussed the Bayes ratio $\frac{p(y| M_1)}{p(y| M_2)}$ as a tool to decide between models.

Here we look at two other approaches to compare models that do not need computing the evidence.

Deviance information criterion (DIC)

The deviance information criterion (DIC) is defined as $$ \text{DIC} = -2\left(\log p(\vec y |\vec\theta^*) - p_\mathrm{D}\right) \ , $$ with the number of effective model parameters $$ p_\mathrm{D} = 2\left(\log p(\vec y |\vec\theta^*) - \E_{p(\theta |\vec y)}[\log p(\vec y |\vec\theta)]\right)\ , $$ where the last term is the mean of the log likelihood over the posterior.

An alternative estimate of the number of effective model parameteres is $$ p_\mathrm{V} = 2\Var_{p(\theta |\vec y)}[\log p(\vec y |\vec\theta)]\,. $$

Interpretation: log-likelihood at the point of the best-fit parameter $\vec\theta^*$ minus the number of parameters in the model.

The better the fit, the higher the likelihood. The DIC is lower for better models, but adding more parameters that do not significantly improve the likelihood are penalised.

Why are p_D and p_V estimates of the effective number of model parameters?

Let us consider the case where the likelihood, posterior, and prior are approximately Gaussian, with d model parameters.

Define $D(\theta) = -2\log p(\vec y |\vec\theta)$. First, expand around the best-fit $\vec\theta^*$: $$ D(\theta) \approx D(\theta^*) + (\theta - \theta^*)D'_{\theta^*} + \frac{1}{2}(\theta - \theta^*)^T D''_{\theta^*}(\theta - \theta^*)\,, $$ where D'_{θ^*} and D''_{θ^*} are the first and second derivatives of D with respect to $\vec\theta$ at $\vec\theta^*$.

Then take the expectation with respect to the posterior: $$ \begin{split} \E[D(\theta)] &\approx D(\theta^*) + E[(\theta - \theta^*)^T D''_{\theta^*}(\theta - \theta^*)] \\ &= D(\theta^*) + \mathrm{tr}(D''_{\theta^*}E[(\theta - \theta^*)(\theta - \theta^*)^T]) \\ &= D(\theta^*) + \mathrm{tr}(D''_{\theta^*}\Sigma_{p(\theta|y)})\,, \end{split} $$ where $\Sigma_{p(\theta|y)}$ is the covariance of the posterior.

Remember the definition of p_D: $$ p_\mathrm{D} = D(\theta^*) - \E[D(\theta)] \approx \mathrm{tr}(D''_{\theta^*}\Sigma_{p(\theta|y)}) $$

We can write $D(\theta)$ in terms of the posterior and prior using Bayes' theorem: $$ D(\theta) = -2\log p(\vec y |\vec\theta) = -2 \log\left(\frac{p(\theta |\vec y)}{p(\vec\theta)} p(\vec y)\right)\,. $$

The Hessian of D''_{θ^*} can now be written as $$ D''_{\theta^*, ij} = -2 \frac{\partial^2}{\partial\theta_i\partial\theta_j}\log p(\theta |\vec y) + 2 \frac{\partial^2}{\partial\theta_i\partial\theta_j}\log p(\theta) \approx \Sigma_{p(\theta|y)}^{-1} - \Sigma_{p(\theta)}^{-1}\,, $$ where we assumed the posterior and prior are Gaussian, with covariances $\Sigma_{p(\theta|y)}$ and $\Sigma_{p(\theta)}$.

Putting things together, we find the effective number of model parameters $$ p_\mathrm{D} \approx \mathrm{tr}(D''_{\theta^*}\Sigma_{p(\theta|y)}) \approx d - \mathrm{tr}(\Sigma_{p(\theta)}^{-1}\Sigma_{p(\theta|y)}) $$ This behaves as we would hope:

- In the case where the prior is very uninformative ($\Sigma_{p(\theta)}\to\infty$) all parameters are constrained by the data: $p_\mathrm{D} = d$.
- In the case where the prior is the same as the posterior ($\Sigma_{p(\theta)} = \Sigma_{p(\theta|y)}$), none of the parameters are constrained by the data: $p_\mathrm{D} = 0$.

Implement the DIC:

```
def DIC(theta_star, theta_samples, log_likelihood):
    # Compute log likelihood at theta_star and the samples theta_i
```

```
    log_likelihood_star = log_likelihood(theta_star)
    log_likelihood_samples = np.array(
        [log_likelihood(theta) for theta in theta_samples]
    )
    p_D = 2*(log_likelihood_star - np.mean(log_likelihood_samples))
    p_V = 2*np.var(log_likelihood_samples)
    return -2*(log_likelihood_star - p_D), p_D, p_V
```

```
DIC_lin, p_D_lin, p_V_lin = DIC(
    theta_star=results_linear["MAP"],
    theta_samples=results_linear["PPD_params"],
    log_likelihood=lambda theta: log_likelihood_lin(y, theta, x, y_err)
)

DIC_quad, p_D_quad, p_V_quad = DIC(
    theta_star=results_quadratic["MAP"],
    theta_samples=results_quadratic["PPD_params"],
    log_likelihood=lambda theta: log_likelihood_quad(y, theta, x, y_err)
)
print(f"Linear: DIC = {DIC_lin:.1f}, p_D = {p_D_lin:.1f}, p_V = {p_V_lin:.1f}")
print(f"Quadratic: DIC = {DIC_quad:.1f}, p_D = {p_D_quad:.1f}, p_V = {p_V_quad:.1f}")
```

```
Linear: DIC = -60.2, p_D = 1.9, p_V = 2.0
Quadratic: DIC = -69.4, p_D = 3.1, p_V = 2.9
```

The quadratic model has a lower DIC and is therefore preferred. The much better fit is not offset my the larger number of parameters.

WAIC

The DIC is easy to calculate but has the downside that it relies on a point estimate for $\vec\theta^*$. A more Bayesian information criterion is the Watanabe-Akaike or widely applicable information criterion (WAIC).

It assumes we can partition the data into M partitions, for example the n entries y_i in the data vector $\vec y$. Then the log pointwise predictive density (lppd) is $$ \text{lppd} = \sum_{i=1}^n\log\E[p(y_i |\vec\theta)] = \sum_{i=1}^n\log\int p(y_i |\vec\theta)p(\vec\theta|\vec y)\dd \theta^n $$

The number of parameters are estimated as $$ p_\mathrm{WAIC} = \sum_{i=1}^n \Var[\log p(\vec y_i |\vec\theta)] $$

Finally, the WAIC is calculated as $$ \text{WAIC} = -2\left(\text{lppd} - p_\mathrm{WAIC}\right) $$

```
def WAIC(theta_samples, log_likelihood, y_partitions, x_partitions, y_err_partitons):
    # Compute the log likelihood for each partition separately
    pointwise_log_likelihood_samples = np.array(
        [[log_likelihood(y_partitions[i], theta, x_partitions[i], y_err_partitons[i])
            for i in range(len(y_partitions))]
         for theta in theta_samples]
    )
```

```
    # Compute the lppd and p_waic for each partition
    lppd = np.log(np.mean(np.exp(pointwise_log_likelihood_samples), axis=0))
    p_waic = np.var(pointwise_log_likelihood_samples, axis=0)
    # Check if the any of the terms in p_waic are too large, which indicates
    # a problem
    if np.any(p_waic > 0.4):
        print(f"Warning: Var[log p(y_i|theta)] > 0.4 for data points "
              f"{np.argwhere(p_waic > 0.4)}. p_WAIC unreliable!")
    # Sum up the partitions
    lppd = np.sum(lppd)
    p_waic = np.sum(p_waic)

    return -2*(lppd - p_waic), p_waic, pointwise_log_likelihood_samples
```

```
WAIC_lin, p_WAIC_lin, pointwise_log_likelihood_samples_lin = WAIC(
    theta_samples=results_linear["PPD_params"],
    log_likelihood=log_likelihood_lin,
    y_partitions=y,
    x_partitions=x,
    y_err_partitons=y_err
)

WAIC_quad, p_WAIC_quad, pointwise_log_likelihood_samples_quad = WAIC(
    theta_samples=results_quadratic["PPD_params"],
    log_likelihood=log_likelihood_quad,
    y_partitions=y,
    x_partitions=x,
    y_err_partitons=y_err
)
print(f"Linear: WAIC = {WAIC_lin:.1f}, p_WAIC = {p_WAIC_lin:.1f}")
print(f"Quadratic: WAIC = {WAIC_quad:.1f}, p_WAIC = {p_WAIC_quad:.1f}")
```

```
Warning: Var[log p(y_i|theta)] > 0.4 for data points [[ 2]
 [29]]. p_WAIC unreliable!
Warning: Var[log p(y_i|theta)] > 0.4 for data points [[25]
 [29]]. p_WAIC unreliable!
Linear: WAIC = -57.7, p_WAIC = 4.0
Quadratic: WAIC = -67.7, p_WAIC = 4.2
```

The WAIC also prefers the quadratic model. Warnings and oddly high number of parameters should give us pause, however.

Cross-validation

Both the DIC and WAIC are approximations to leave-one-out cross-validation (LOO-CV).

The idea behind cross-validation is to split the data into a training set y_train and a holdout set y_holdout.

We then evaluate the PPD (using the posterior $p(\theta | y_\mathrm{train})$) at y_holdout.

This checks if the model can predict each data point given all the other data points.

More specifically, we split the data into n partions and for each compute $$ \log \int p(y_{i} | \theta)p(\theta | y_{(-i)}) \dd \theta\ , $$ where y_i is the partion i of the data and $y_{(-i)}$ is the data without the partion i.

This becomes computationally expensive quickly, since for each partion we need to create samples from the posterior $p(\theta | y_{(-i)})$. It also explicitly requires the data to be able to be split into partitions, which might be difficult for structured or dependent data.

A sophisticated approximation to LOO-CV that avoids recalculating the posterior for the partions is implemented in the package `arviz`. It also implements WAIC and other statistical diagnostics, for example for MCMC.

```
import arviz

inference_data_lin = arviz.from_dict(
    posterior={"lin": results_linear["PPD_params"][None, ...]},
    log_likelihood={"lin": pointwise_log_likelihood_samples_lin[None, ...]},
)

inference_data_quad = arviz.from_dict(
    posterior={"quad": results_quadratic["PPD_params"][None, ...]},
    log_likelihood={"quad": pointwise_log_likelihood_samples_quad[None, ...]},
)
arviz.compare({"lin": inference_data_lin, "quad": inference_data_quad}, ic="loo", sca
```

	rank	elpd_loo	p_loo	elpd_diff	weight	se	dse	warning	scale
quad	0	-66.855284	4.660655	0.000000	0.793203	8.325738	0.000000	False	deviance
lin	1	-57.497176	4.131351	9.358108	0.206797	14.849195	9.453856	False	deviance

Supernovae

Let us apply the goodness-of-fit tests and DIC to the supernova example!

First, the chi-squared test:

```
n_data = len(data)
n_param_flat_lcdm = 3
n_param_lcdm = 4

chi_squared_flat_lcdm = -2*log_likelihood_flat_LCDM(theta_MAP_flat_lcdm)
chi_squared_lcdm = -2*log_likelihood_LCDM(theta_MAP_lcdm)

PTE_flat_lcdm = scipy.stats.chi2(df=n_data - n_param_flat_lcdm).sf(chi_squared_linear)
PTE_lcdm = scipy.stats.chi2(df=n_data - n_param_lcdm).sf(chi_squared_quadratic)

print(f"Flat LCDM: χ²={chi_squared_flat_lcdm:.2f}, "
```

```
      f"ndof={n_data}-{n_param_flat_lcdm}, PTE={PTE_flat_lcdm:.3f}")

print(f"LCDM: χ²={chi_squared_lcdm:.2f}, "
      f"ndof={n_data}-{n_param_lcdm}, PTE={PTE_lcdm:.3f}")
```

```
Flat LCDM: χ²=1441.69, ndof=1580-3, PTE=1.000
LCDM: χ²=1441.41, ndof=1580-4, PTE=1.000
```

The χ^2 values are too low for the number of data points. This suggests that the data uncertainties are overestimated. Let us run an MCMC chain (with `zeus` in this case) and look at the PPD test statistic.

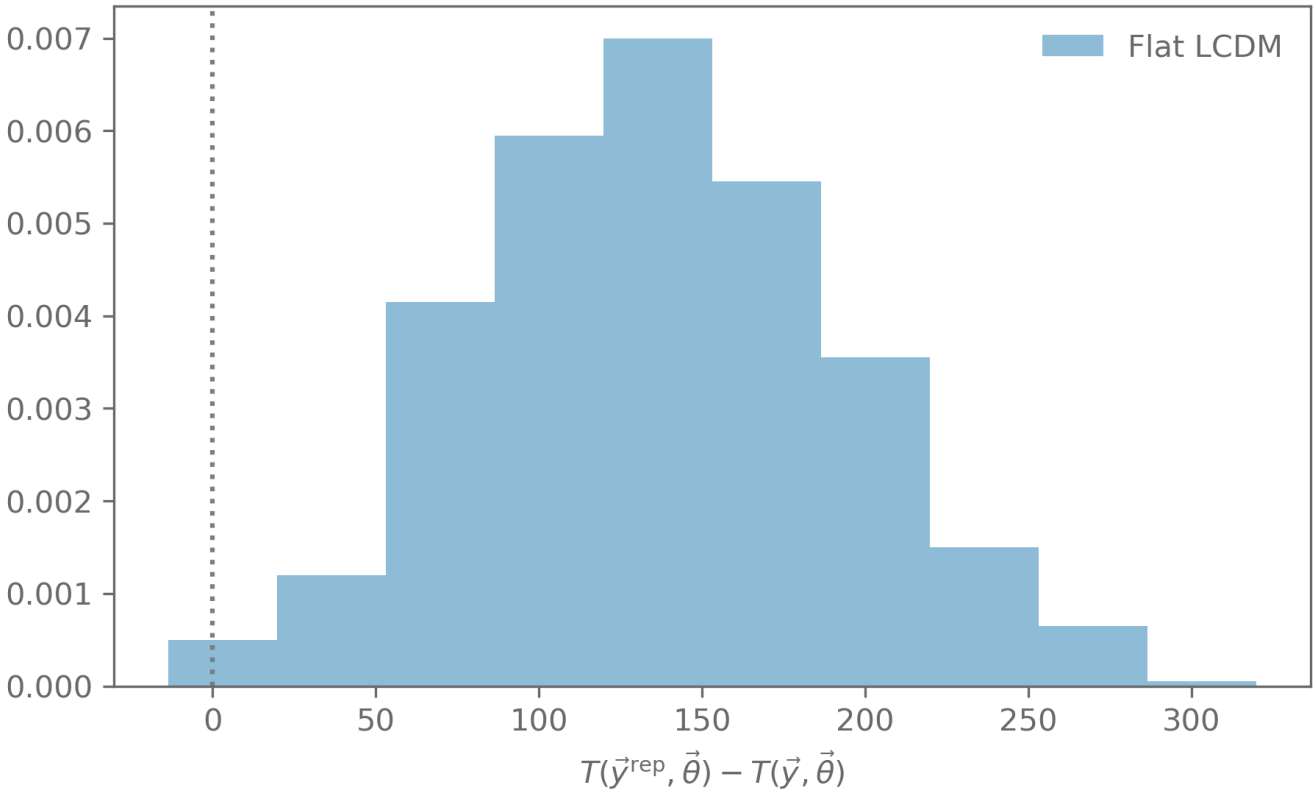
```
import zeus

n_param = 4
n_walker = 12
n_step = 100

start_point = np.random.normal(size=(n_walker, n_param), loc=theta_MAP_lcdm, scale=(0.

sampler_lcdm = zeus.EnsembleSampler(nwalkers=n_walker, ndim=n_param, logprob_fn=log_po

sampler_lcdm.run_mcmc(start=start_point, nsteps=n_step, progress=True)

print("Integrated autocorrelation time:", zeus.AutoCorrTime(sampler_lcdm.get_chain()))

chain_lcdm = sampler_lcdm.get_chain(discard=50, flat=True)
```

```
Initialising ensemble of 12 walkers...
Sampling progress : 100%|██████████| 100/100 [00:28<00:00,  3.50it/s]
Integrated autocorrelation time: [5.44045274 4.71651602 5.50330958 7.05414514]
```

We use the χ^2 as the test statistic again:

```
def test_statistic(data, mu):
    r = data - mu
    return r @ inv_covariance @ r

T_rep_flat_lcdm = np.array([
    test_statistic(
        data=sample_from_likelihood_flat_LCDM(p),
        mu=flat_LCDM_distance_modulus_model(p, z_data)
    ) for p in chain_flat_lcdm
])
T_flat_lcdm = np.array([
    test_statistic(
        data=data,
        mu=flat_LCDM_distance_modulus_model(p, z_data)
    ) for p in chain_flat_lcdm
])

ppd_pte_flat_lcdm = (T_rep_flat_lcdm > T_flat_lcdm).sum()/T_rep_flat_lcdm.size

print(f"Flat LCDM PPD PTE: {ppd_pte_flat_lcdm:.3f}")
```

```
Flat LCDM PPD PTE: 0.995
```



This also indicates that the observed data do not scatter as much as our model suggests.

Something is not right. The first suspect is the data covariance.

We used the STAT+SYS covariance here. That means the covariance includes the systematic uncertainty on top of the statistical uncertainty. This could explain the very high PTE on the test statistic.

We already compared the flat and non-flat ΛCDM models using the Bayes' ratio. Now er see what the DIC tells us:

```
DIC_flat_lcdm, p_D_flat_lcdm, p_V_flat_lcdm = DIC(
    theta_star=theta_MAP_flat_lcdm,
    theta_samples=chain_flat_lcdm,
    log_likelihood=log_likelihood_flat_LCDM
)
DIC_lcdm, p_D_lcdm, p_V_lcdm = DIC(
    theta_star=theta_MAP_lcdm,
    theta_samples=chain_lcdm,
    log_likelihood=log_likelihood_LCDM
)

print(f"Flat LCDM: DIC = {DIC_flat_lcdm:.1f}, p_D = {p_D_flat_lcdm:.1f}, p_V = {p_V_f
print(f"LCDM: DIC = {DIC_lcdm:.1f}, p_D = {p_D_lcdm:.1f}, p_V = {p_V_lcdm:.1f}")
```

```
Flat LCDM: DIC = 1446.1, p_D = 2.2, p_V = 2.0
LCDM: DIC = 1447.5, p_D = 3.1, p_V = 3.5
```

The DIC slightly prefers the simpler, flat ΛCDM model.

We also see that the estimates of the number of model parameters makes sense: the flat ΛCDM model has 3 parameters (H_0, Ω_m, M) but H_0 is completly constrained by the prior. So effectively, the data can only inform ≈ 2 parameters.

The non-flat model has 4 parameters but again, H_0 is completly constrained by the prior, so we are left with ≈ 3 effective free parameters.

Exercise

Reproduce the chi-squared and PPD-based test with your own analysis code.

Show that for a Gaussian posterior with a wide and uniform prior, the estimate p_V of the effective number of free parameters reduces to the dimensionality of the Gaussian.

Try a cubic model. What are the DIC, WAIC, and Bayes factor?