Tutorial 9

Statistical Computation and Analysis

Spring 2025

Tutorial Outline

- Model comparison
  - Widely applicable information criteria
  - Cross validation
- Model averaging

Model Comparison

- How can we compare two or more models for the same data?
  - We have used posterior predictive checks to assess how well a model explains the data used to fit a model.
  - We have looked at Bayesian p values.
  - Now we'll learn additional methods for comparing between models.

Model Comparison

- We aim for:
  - High goodness of fit
    - Model fits the data
  - Lower complexity
    - Fewer parameters (more parameters can lead to overfitting)
  - High generalizability
    - Model predicts future data well

Model Comparison

- Within-sample accuracy :
  - The accuracy is measured with the same data used to fit the model.
- Out-of-sample accuracy :
  - The accuracy measured with data not used to fit the model.
- The within-sample accuracy will be higher and lead us to believe our model is better than it is.
- Leaving data out means less data to fit our model.

Model Comparison

- To overcome this, we will use two methods:
  - **Information criteria:** Expressions that approximate out-of-sample accuracy as in-sample accuracy plus a term that penalizes model complexity.
  - **Cross-validation:** A method that involves dividing the available data into separate subsets that are alternatively used to fit and evaluate the models

Widely Applicable Information Criteria

$$WAIC = \underbrace{-2\sum_{i}^{n}\log\left(\frac{1}{S}\sum_{s=1}^{S}p(y_i \mid \theta^s)\right)}_{\text{A measure of how well the model fits the data}} + \underbrace{2\sum_{i}^{n}\left(V_{s=1}^{S}\log p(y_i \mid \theta^s)\right)}_{\text{A measure of the effective number of parameters}}$$

- **We will choose the model with the lower WAIC.**
- The second term corrects for how much the likelihood would change if we had new data.
  - If two models fit the data equally well, we will choose the simpler one.

Cross Validation

- Divide our data into k parts.
- Use k-1 parts to fit the model and test it on the left-out portion.
- We get k models and k accuracy values.
- The accuracy of the model is the average of the k accuracy values.
- Fit the model on all the data one final time.
  - This is the final model for future use.

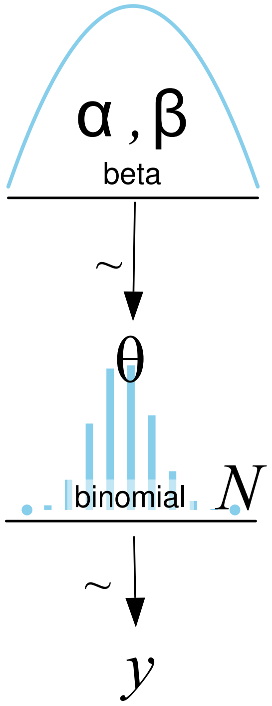
Cross Validation

- When K equals the number of data points, we get what is known as **leave-one-out cross validation (LOOCV)**, meaning we fit the model to all but one data point each time.
- Practically, this is computationally expensive, and we are going to estimate it.

Null and Alternative Model

- Null model: coin is fair.
- Alternative model: coin is biased.

Graphical model



PyMC (a PPL)

```
coords = {"data": np.arange(len(data))}

with pm.Model(coords=coords) as model_1:
    thet = pm.Beta('thet', alpha=1., beta=1.)
    y = pm.Bernoulli('y', p=thet, observed=data, dims = 'data')
    idata1 = pm.sample(1000, chains = 4, idata_kwargs={"log_likelihood":True})
```

arviz.InferenceData

- ▸ posterior
- ▸ log_likelihood
- ▸ sample_stats
- ▸ observed_data

Null and Alternative Model

- First, let's look at the WAIC and LOO of our model:

```
az.waic(idata1)
```

	0
elpd_waic	-60.260962
se	4.245041
p_waic	0.961681
n_samples	4000
n_data_points	100
warning	False
waic_i	[<xarray.DataArray 'waic_i' ()> Size: 8B\narra...
scale	log

```
print(az.loo(idata1))
```

```
Computed from 4000 posterior samples and 100 observations log-likelihood matrix.

         Estimate       SE
elpd_loo   -60.26     4.25
p_loo        0.96        -
------

Pareto k diagnostic values:
                         Count   Pct.
(-Inf, 0.70]   (good)      100  100.0%
   (0.70, 1]   (bad)         0    0.0%
   (1, Inf)   (very bad)    0    0.0%
```

Effective number of parameters

How reliable is our estimate?
Values above 0.7 indicate that we may have very influential datapoints – bad.
We can see that 100% of our datapoints are good.

- Now let's compare the values to those of the null model.

Null and Alternative Model

```
# Compare
az.compare({"alternative": idata1, "null": idata_null})
```

From best to worst

Higher = better

	rank	elpd_loo	p_loo	elpd_diff	weight	se	dse	warning	scale
alternative	0	-60.263062	0.963782	0.000000	0.94854	4.245280	0.000000	False	log
null	1	-65.995594	0.193007	5.732533	0.05146	0.800336	3.444944	False	log

If the difference between the elpd values is bigger

than the standard error

Then we say that there is a meaningful difference between the two models

Null and Alternative Model

- That was the LOO values, now we can do the same with the widely accepted information criteria.

```
# Compare WAIC
az.compare({"alternative": idata1, "null": idata_null}, ic = 'waic')
```

	rank	elpd_waic	p_waic	elpd_diff	weight	se	dse	warning	scale
alternative	0	-60.260962	0.961681	0.000000	0.948718	4.245041	0.000000	False	log
null	1	-65.995353	0.192766	5.734392	0.051282	0.800333	3.444707	False	log

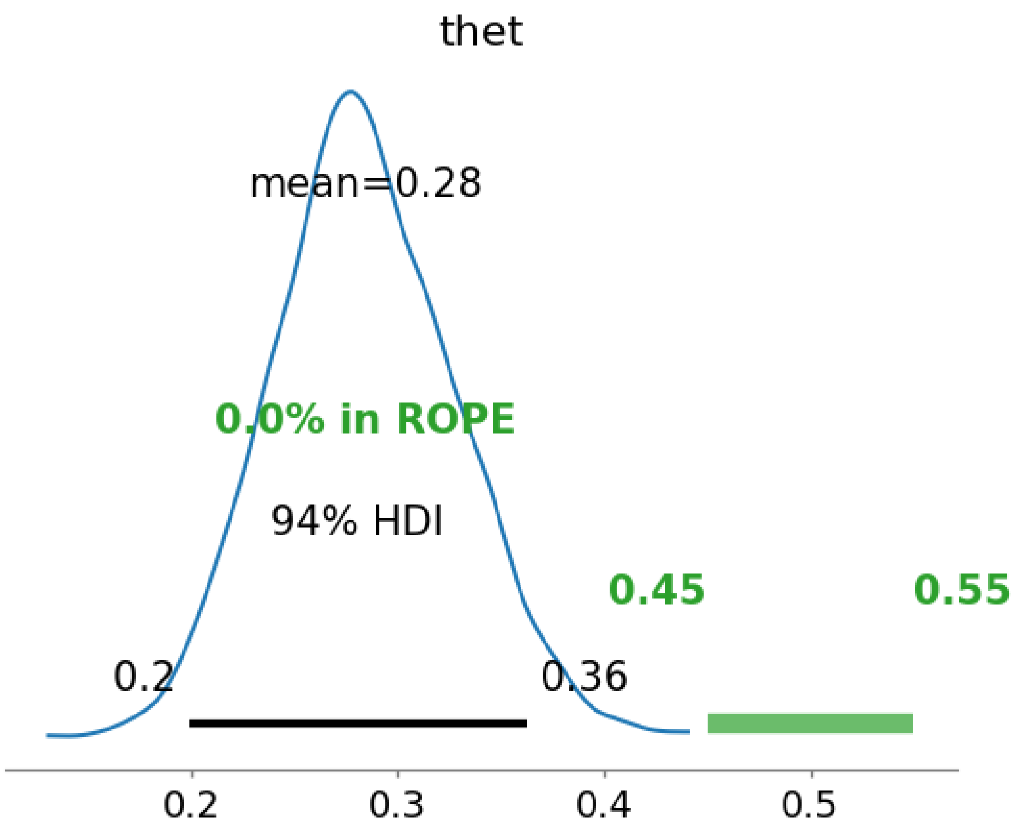
- The WAIC and LOO values are generally almost exactly the same.
  - At this point, it is generally more accepted to use the LOO.

Null and Alternative Model

- We created the null model by using a very narrow posterior defined by the ROPE.
- We defined the ROPE as [0.45, 0.55].
- Another option for comparison is to check if the HDI and ROPE overlap.
- Based on our model comparison using LOO and WAIC, we concluded that there is a meaningful difference between the null and alternative models.

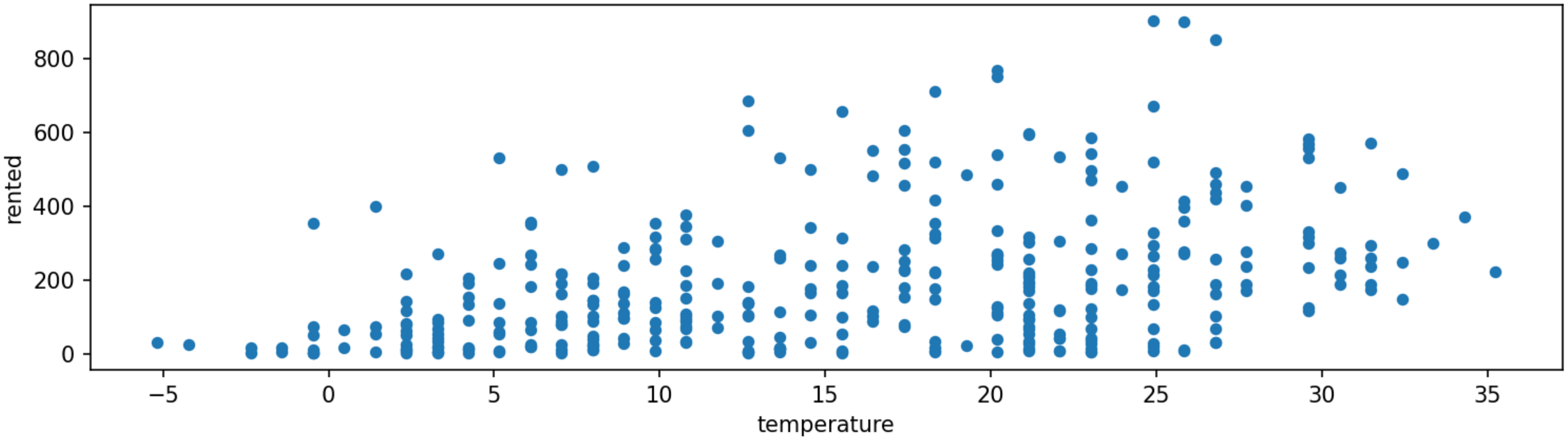
Null and Alternative Model

- We arrive at the same conclusion looking at the HDI and ROPE
  - There is no overlap between them
  - We reject the null model of a fair coin



Bikes Example

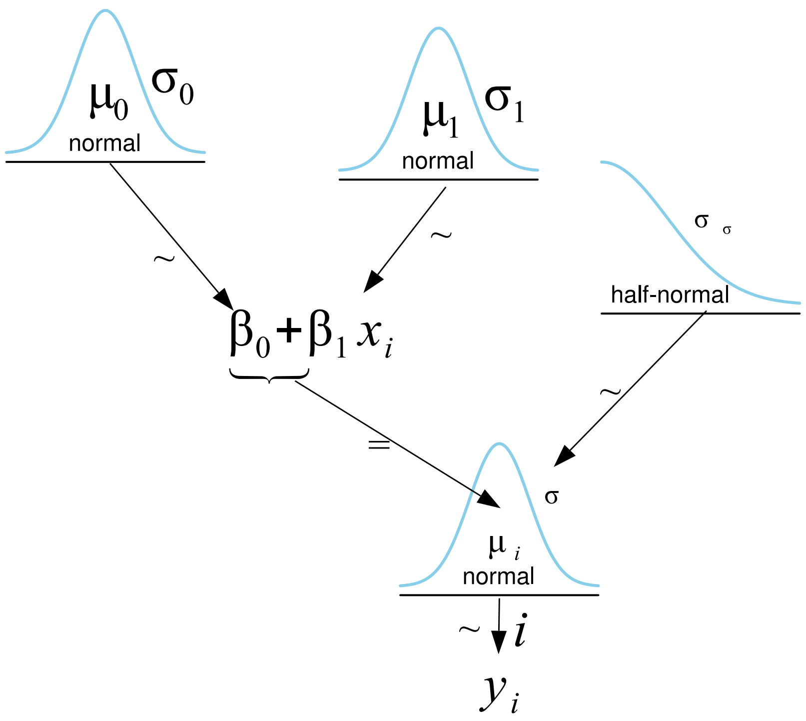
- In the lecture, you looked at bike rentals as a function of temperature using several models:



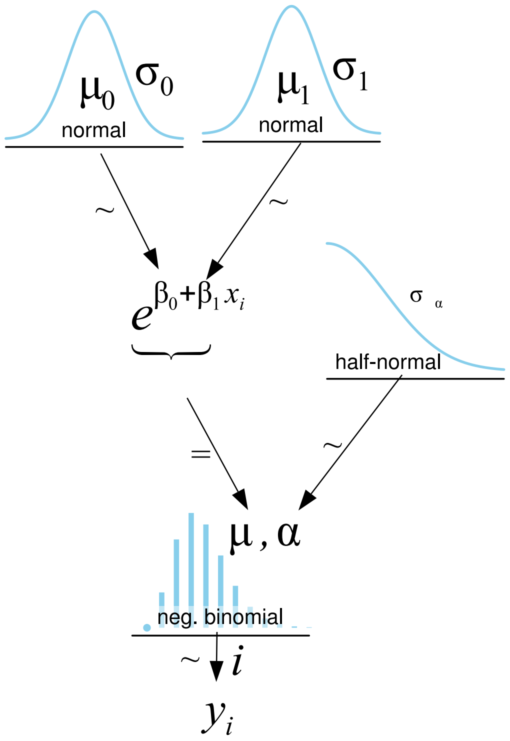
Bikes Example

- In the lecture, you looked at bike rentals as a function of temperature using two models:

Linear Model



Negative Binomial Model



Bikes Example

- In the lecture, you looked at bike rentals as a function of temperature using two models:

Linear Model

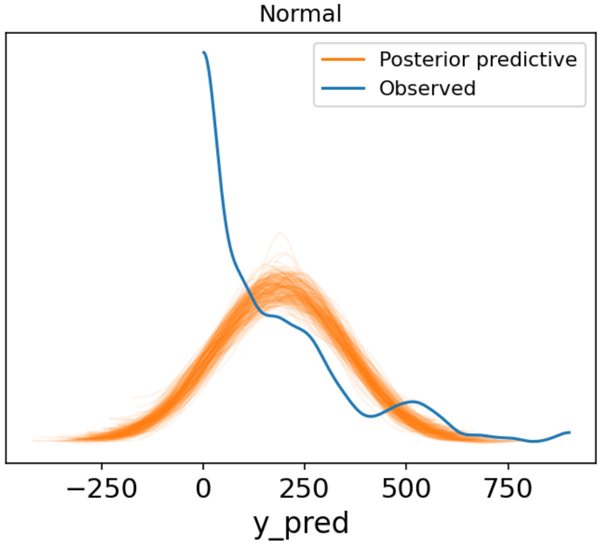
```
coords = {"data": np.arange(len(bikes))}
with pm.Model(coords=coords) as model_lb:
    β0 = pm.Normal("β0", mu=0, sigma=100)
    β1 = pm.Normal("β1", mu=0, sigma=10)
    σ = pm.HalfNormal("σ", 10)
    μ = pm.Deterministic("μ", β0 + β1 * bikes.temperature, dims="data")
    y_pred = pm.Normal("y_pred", mu=μ, sigma=σ, observed=bikes.rented, dims="data")
    idata_lb = pm.sample(1000, chains = 4, idata_kwargs={"log_likelihood":True})
```

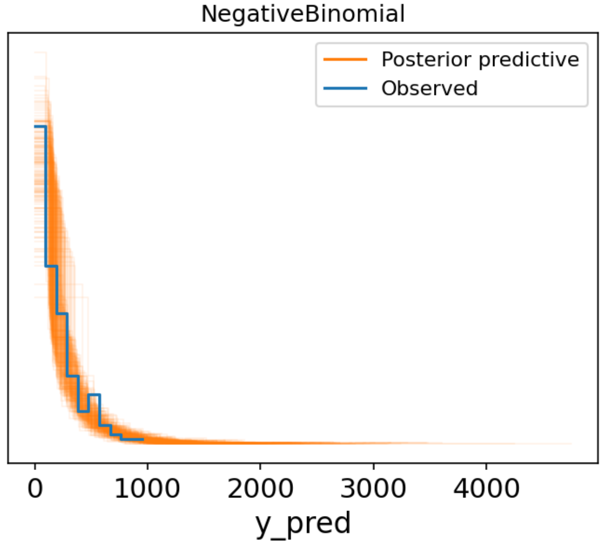
Negative Binomial Model

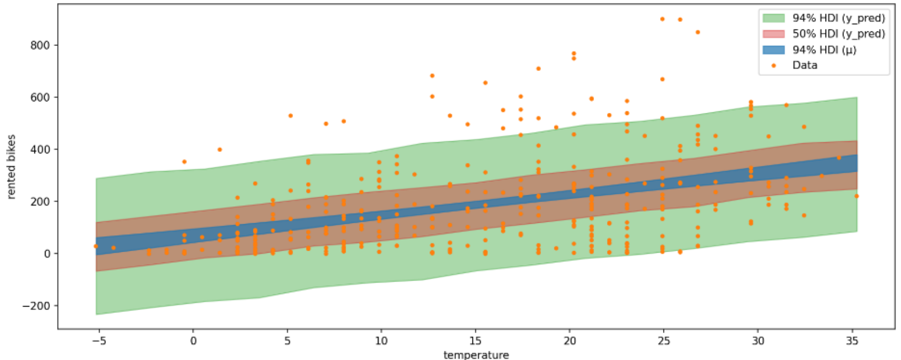
```
with pm.Model() as model_neg:
    beta0 = pm.Normal("beta0", mu=mu_0, sigma=sigma_0)
    beta1 = pm.Normal("beta1", mu=mu_1, sigma=sigma_1)
    alpha = pm.HalfNormal("alpha", sigma=sigma_alpha)
    mu = pm.Deterministic("mu", pm.math.exp(beta0 + beta1 * bikes.temperature))
    y_pred = pm.NegativeBinomial("y_pred", mu=mu, alpha=alpha, observed=bikes.rented)
    idata_neg = pm.sample(1000, chains = 4, idata_kwargs={"log_likelihood":True})
```

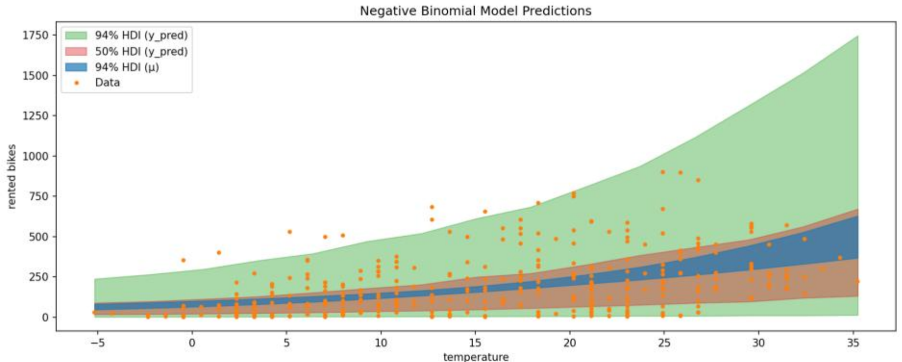
Bikes Example

- In the lecture you compared the two using posterior predictive checks and saw that the negative binomial model was better:









Bikes Example

- Let's add the WAIC and LOO to the comparison:

	rank	elpd_loo	p_loo	elpd_diff	weight	se	dse	warning	scale
negative_binomial	0	-2153.169315	2.742507	0.000000	1.0	19.804978	0.000000	False	log
linear	1	-2300.275960	4.858970	147.106645	0.0	26.995013	21.713316	False	log

	rank	elpd_waic	p_waic	elpd_diff	weight	se	dse	warning	scale
negative_binomial	0	-2153.163883	2.737075	0.000000	1.0	19.804702	0.000000	False	log
linear	1	-2300.267411	4.850421	147.103528	0.0	26.993311	21.711993	True	log

Bikes Example

- We also learned about multiple regression.
- Another use for model comparison can be to test the value of adding additional independent variables.
  - Adds information to the model.
  - Adds complexity.
- We can add another independent variable of the humidity of the day.

Bikes Example

- Create and sample:

```
with pm.Model() as model_mlb:
    α = pm.Normal("α", mu=0, sigma=1)
    β0 = pm.Normal("β0", mu=0, sigma=10)
    β1 = pm.Normal("β1", mu=0, sigma=10)
    σ = pm.HalfNormal("σ", 10)
    μ = pm.Deterministic("μ", pm.math.exp(α + β0 * bikes.temperature + β1 * bikes.humidity))
    _ = pm.NegativeBinomial("y_pred", mu=μ, alpha=σ, observed=bikes.rented)

    idata_mlb = pm.sample(1000, chains = 4, idata_kwargs={"log_likelihood":True})
```

Bikes Example

- Now let's compare all three:

```
az.compare({"linear": idata_lb, "negative_binomial": idata_neg, "negative_binomial_multiple": idata_mlb})
```

	rank	elpd_loo	p_loo	elpd_diff	weight	se	dse	warning	scale
negative_binomial_multiple	0	-2141.148332	3.725948	0.000000	1.000000e+00	20.860020	0.000000	False	log
negative_binomial	1	-2153.169315	2.742507	12.020983	0.000000e+00	19.804978	3.837865	False	log
linear	2	-2300.275960	4.858970	159.127628	2.428169e-11	26.995013	22.536404	False	log

- We can see that the difference between the LOO values for the two negative binomial models is larger than the standard error.
  - We can conclude from this that it is worth adding the humidity despite it leading to a more complex model.

Model Averaging

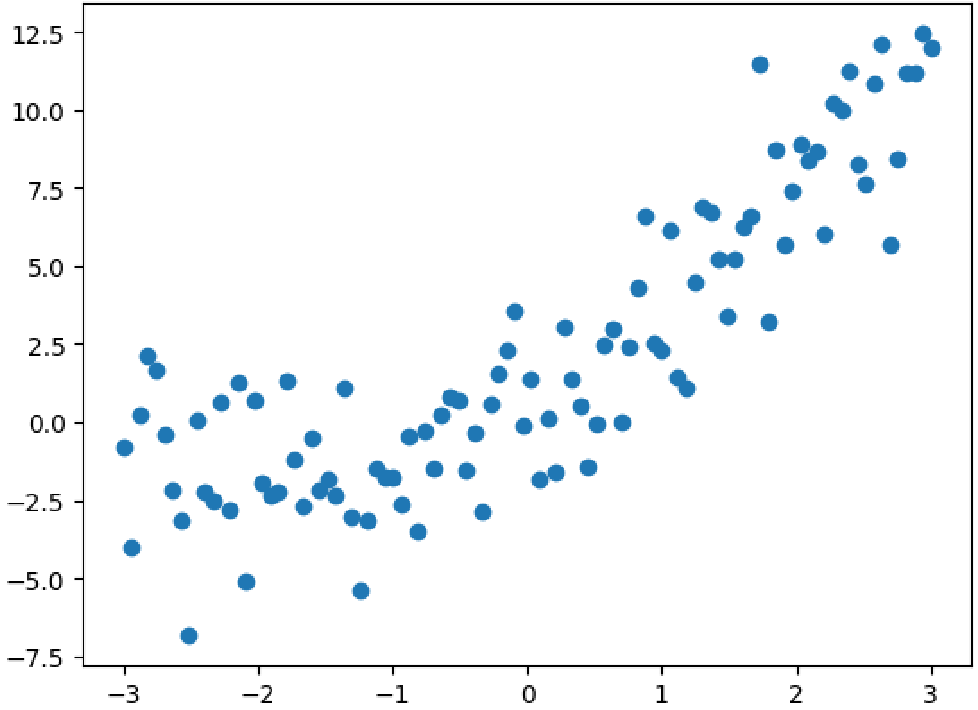
- Instead of choosing one model, we can also average the different models.
- We can compute a weighted average of the different models.
- The weights are computed in the compare function.
  - They are the relative weight of each model and, in large, represent the probability of each model given the data.

```
az.compare({"linear": idata_lb, "negative_binomial": idata_neg, "negative_binomial_multiple": idata_mlb})
```

	rank	elpd_loo	p_loo	elpd_diff	weight	se	dse	warning	scale
negative_binomial_multiple	0	-2141.148332	3.725948	0.000000	1.000000e+00	20.860020	0.000000	False	log
negative_binomial	1	-2153.169315	2.742507	12.020983	0.000000e+00	19.804978	3.837865	False	log
linear	2	-2300.275960	4.858970	159.127628	2.428169e-11	26.995013	22.536404	False	log

Model Averaging

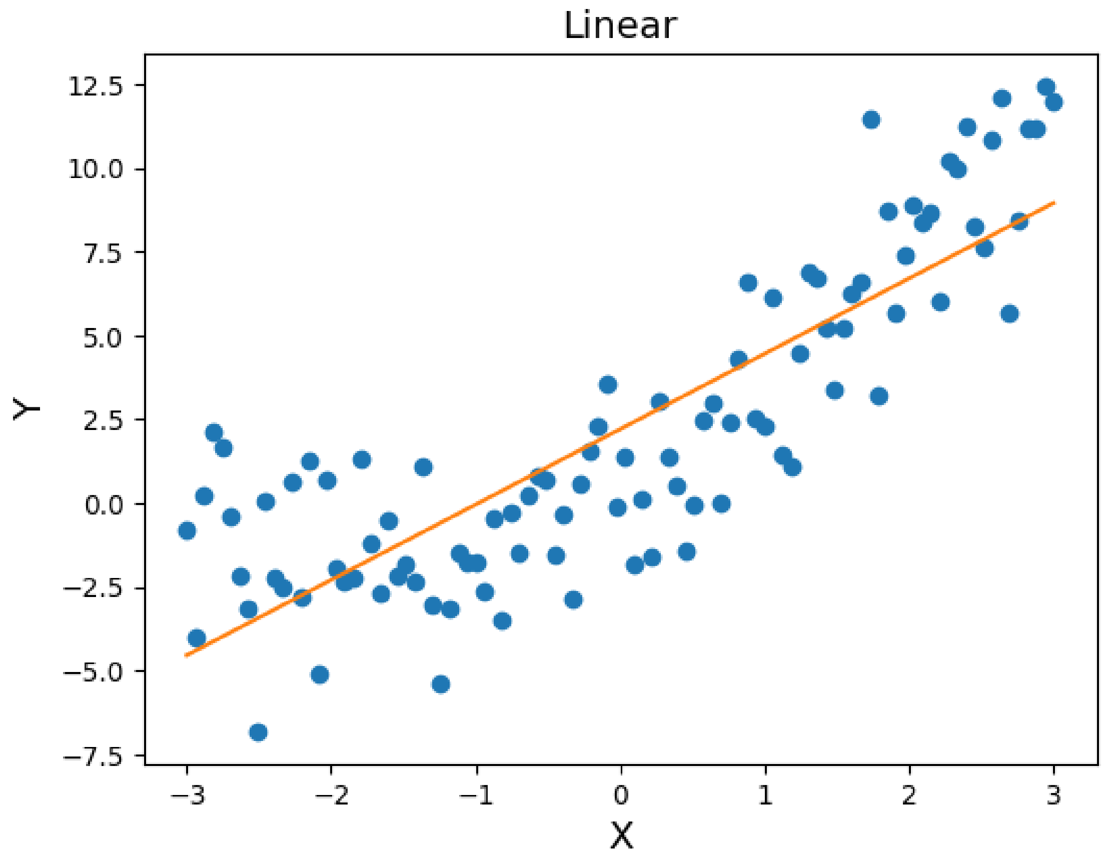
- Let's create random data with two models that give not zero weights.

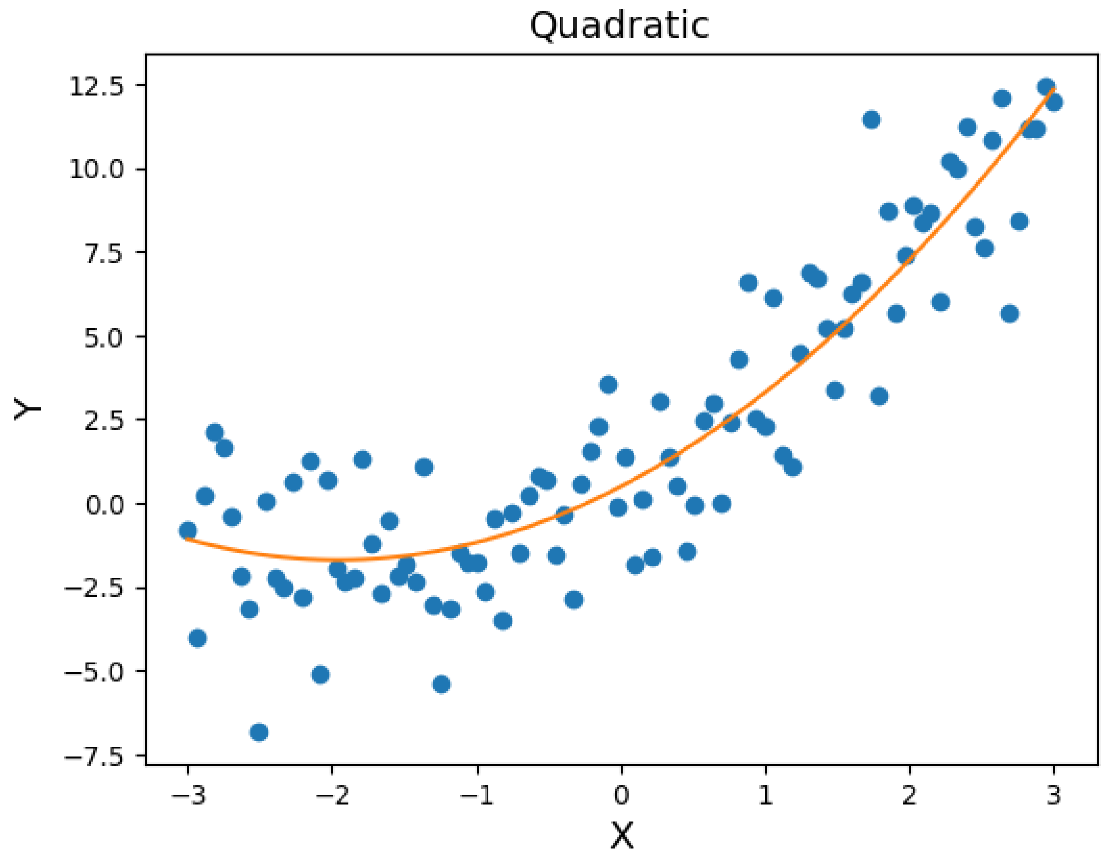


- We'll use a linear model
  - Simpler but fits data less well
- And a quadratic model
  - Fits better but more complex

Model Averaging

- The means of the two models:





Model Averaging

- Comparing between them yields:

```
cmp_df = az.compare({"linear": idata_linear, "quadratic": idata_quad})
cmp_df
```

	rank	elpd_loo	p_loo	elpd_diff	weight	se	dse	warning	scale
quadratic	0	-212.428280	4.036177	0.000000	0.945733	7.300654	0.000000	False	log
linear	1	-236.306868	2.944081	23.878587	0.054267	6.160884	6.660192	False	log

- We will use these weights to compute the weighted average model.

Model Averaging

- Comparing between them yields:

```
cmp_df = az.compare({"linear": idata_linear, "quadratic": idata_quad})
cmp_df
```

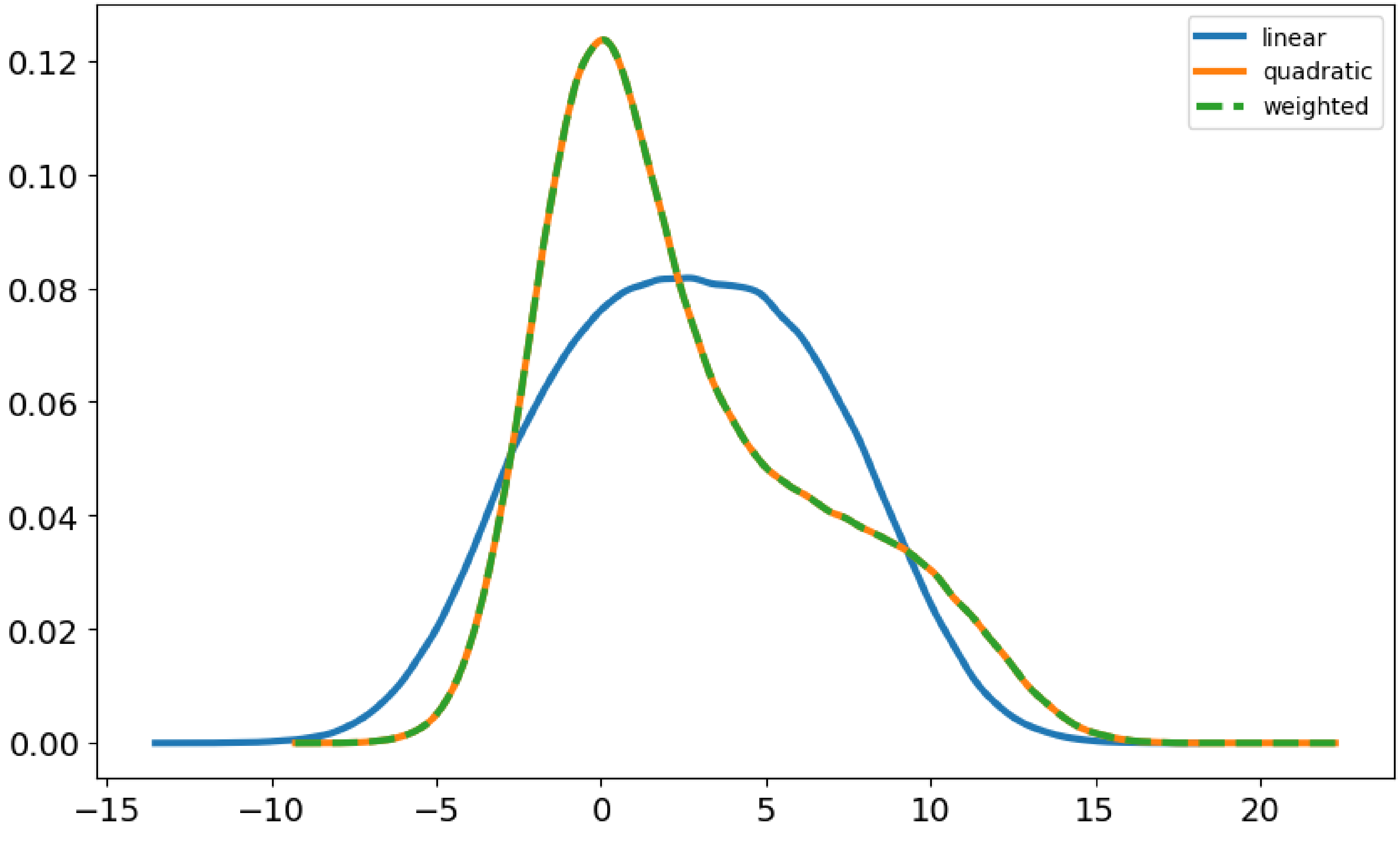
	rank	elpd_loo	p_loo	elpd_diff	weight	se	dse	warning	scale
quadratic	0	-212.428280	4.036177	0.000000	0.945733	7.300654	0.000000	False	log
linear	1	-236.306868	2.944081	23.878587	0.054267	6.160884	6.660192	False	log

- We will use these weights to compute the weighted average model.

```
avg_preds = az.weight_predictions([idata_quad, idata_linear], weights=cmp_df["weight"].values)
```

Model Averaging

- Plotting:



Model Averaging

- We can also define the weights however we like.
  - Example: half to each of the two models.