A guide for fitting generalized linear models in Tensorflow

Shih-Yi Tseng

Harvey Lab, Havard Medical School

Generalized linear model (GLM)

- Flexible generalization of ordinary linear regression
  - Response variable y follows a specific distribution (*noise model*)
  - A function of the mean response variable (*link function*) varies linearly with the predictors X

$$f(\mu) = Xw,\ y \sim \mathrm{Dist}(\mu, \dots)$$

Model type	Distribution	Link function	Mean function (inverse function, activation function)
Linear regression	Normal (Gaussian)	Identity $f(\mu) = \mu$	Linear $\mu = Xw$
Poisson regression	Poisson	Log $f(\mu) = \log(\mu)$	Exponential $\mu = \exp(Xw)$
Logistic regression	Bernoulli	Logit $f(\mu) = \log(\mu/(1 - \mu))$	Sigmoid $\mu = \exp(Xw) / (1 + \exp(Xw))$

Fitting GLM in Tensorflow

- Why Tensorflow?
  - GPU acceleration for massive parallelization
- A typical session with simultaneous recording
  - 200-300 neurons per imaging plane
  - ~30,000 timepoints
  - ~1000 predictors (after basis expansion)

$$\underbrace{f(Y)}_{30{,}000 \times 250} = \underbrace{X}_{30{,}000 \times 1000} \underbrace{W}_{1000 \times 250}$$

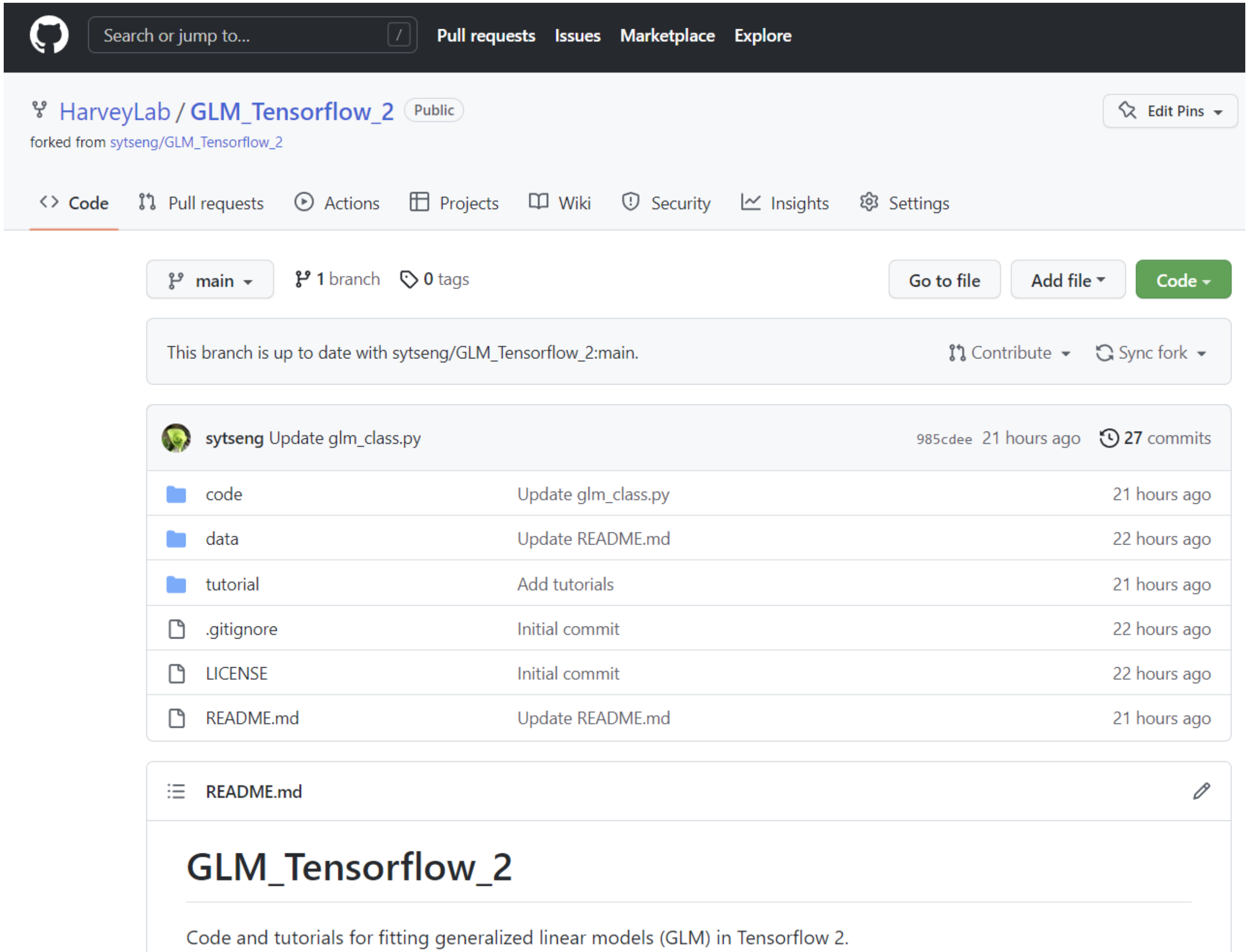
- Formalized as a multi-output, one-layer feedforward neural network
- Combine all outputs for a single loss
- Gradient descent optimization

Fitting takes 5-10 min for Poisson GLMs (1-2 sec per neuron!)

with 5-fold cross validation over >10 regularization values

Github repo for GLM in Tensorflow

https://github.com/HarveyLab/GLM_Tensorflow_2



Tutorials for fitting GLM in Tensorflow

- Two tutorials

  - Tutorial_for_using_GLM_class.ipynb

  - Tutorial_for_fitting_neural_calcium_imaging_data_with_GLM.ipynb

GLM class

- Written in Python, object-oriented
- Can be loaded as a module

```
import glm_class as glm
```

- Initialization

`model = glm.GLM()` or `model = glm.GLM_CV()`

- Four class methods

```
model.fit()
model.select_model()
model.predict()
model.evaluate()
```

Model initialization

```
model = glm.GLM(activation = 'linear', loss_type = 'gaussian',
                regularization = 'elastic_net', lambda_series = 10.0 ** np.linspace(3, -6, 10),
                l1_ratio = 0., smooth_strength = 0.,
                optimizer = 'adam', learning_rate = 1e-2, momentum = 0.5,
                min_iter_per_lambda = 100, max_iter_per_lambda = 10**4,
                num_iter_check = 100, convergence_tol = 1e-6)
```

- Four types of input arguments
  - Model type:
    - *activation:* 'linear', 'exp', 'sigmoid', 'relu', 'softplus'
    - *loss_type:* 'gaussian', 'poisson', 'binominal'
  - Regularization:
    - *regularization:* 'elastic_net', 'group_lasso'
    - *lambda_series:* list of regularization strengths in descending order
    - *l1_ratio:* 0 for L2/ridge, 1 for L1/Lasso, or btw 0-1 for elastic net
    - *smooth_strength:* add smoothness penalty
  - Optimization: *optimizer* ('adam', 'sgdm'), *learning_rate*, *momentum*
  - Convergence: *min_iter_per_lambda, max_iter_per_lambda, num_iter_check, convergence_tol*

Class methods

Fitting (with training data)

```
model.fit(X, Y, [initial_w0, initial_w,
             feature_group_size, verbose])
```

A list containing the size of each group
For group_lasso or smoothness penalty

Model selection (with validation data)

```
model.select_model(X_val, Y_val, [min_lambda, make_fig])
```

Evaluation (with training, validation, and test data)

```
frac_dev_expl, dev_model, dev_null, dev_expl
  = model.evaluate(X, Y, [make_fig])
```

Prediction (with training, validation, and test data)

```
Y_pred = model.predict(X)
```

Model attributes

- Loss & lambda trace

  `model.loss_trace` and `model.lambda_trace`

- Selected weights & intercepts

  `model.selected_w` and `model.selected_w0`

- Selected lambda & lambda indices

  `model.selected_lambda` and `model.selected_lambda_ind`

GLM with cross validation

- Model initialization

```
model_cv = glm.GLM_CV(n_folds = 5, auto_split = True, split_by_group = True, split_random_state = 42,
                      activation = 'linear', loss_type = 'gaussian',
                      regularization = 'elastic_net', lambda_series = 10.0 ** np.linspace(3, -6, 10),
                      l1_ratio = 0., smooth_strength = 0.,
                      optimizer = 'adam', learning_rate = 1e-2, momentum = 0.5,
                      min_iter_per_lambda = 100, max_iter_per_lambda = 10**4,
                      num_iter_check = 100, convergence_tol = 1e-6)
```

- Additional input arguments
  - *n_folds:* number of CV folds
  - *auto_split:* perform CV split automatically
  - *split_by_group:* split CV folds according to a third-party group provided during fitting time
  - *split_random_state:* Numpy random state for splitting

GLM with cross validation

- Model fitting

Train and validation indices for each fold
if *auto_split = False*

Third party group info
if *split_by_group = True*

```
model_cv.fit(X, Y, [train_idx, val_idx, group_idx,
                    initial_w0, initial_w,
                    feature_group_size, verbose])
```

- Model selection (no validation data required)

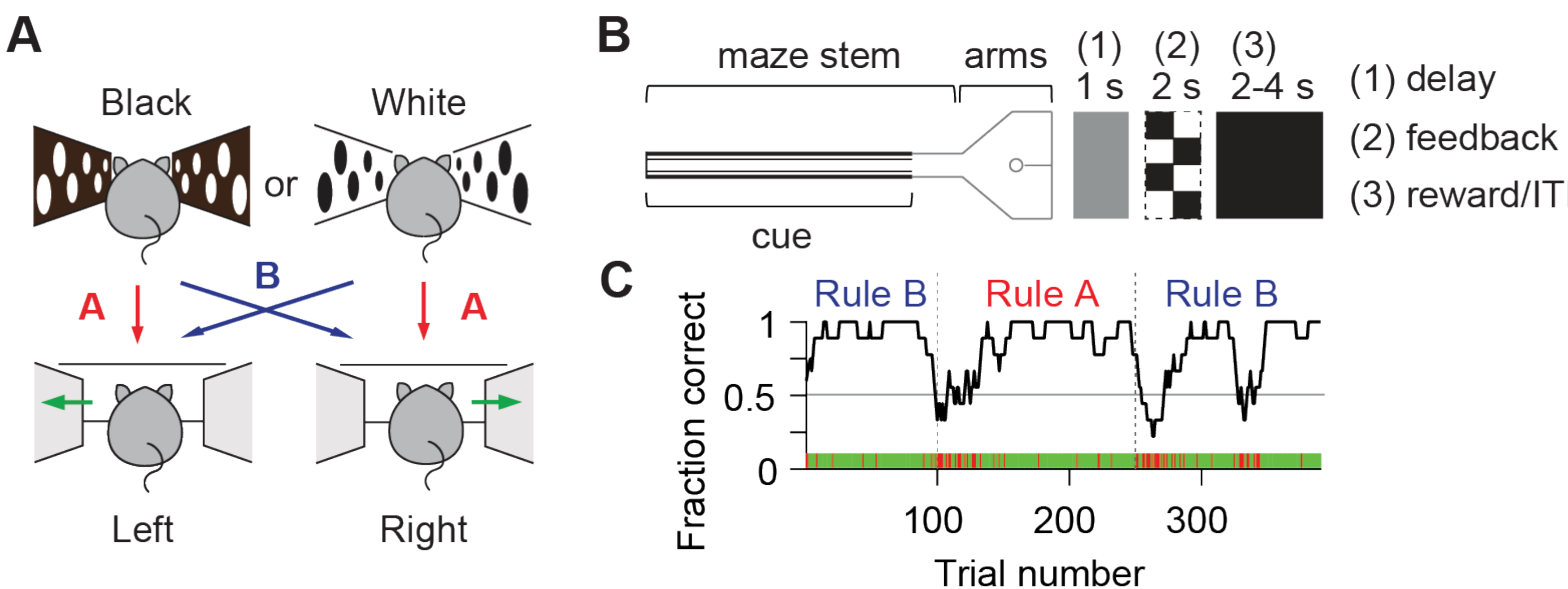
```
model_cv.select_model([se_fraction, min_lambda, make_fig])
```

Controls the tolerance of choosing models with smallest deviance vs. larger regularization;
0 for model with minimal deviance, 1 for 1SE rule

- Same methods for model evaluation and prediction

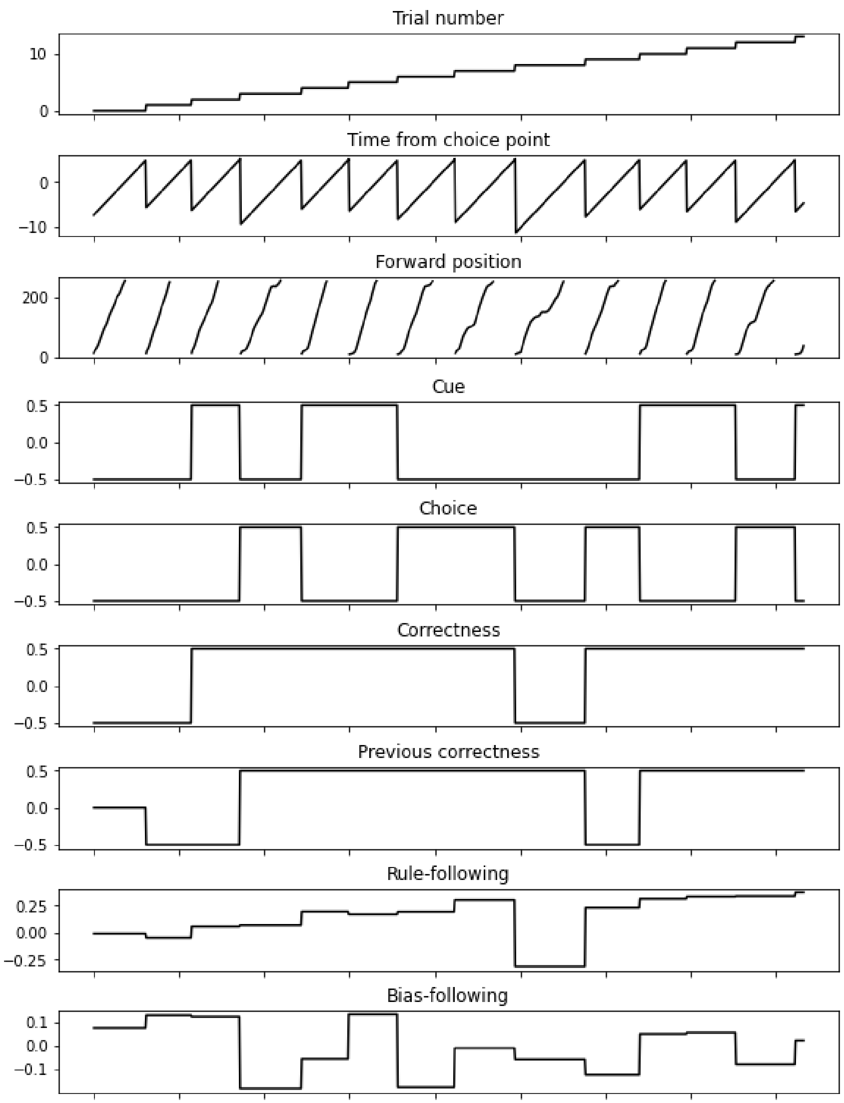
Fitting GLM to calcium imaging data

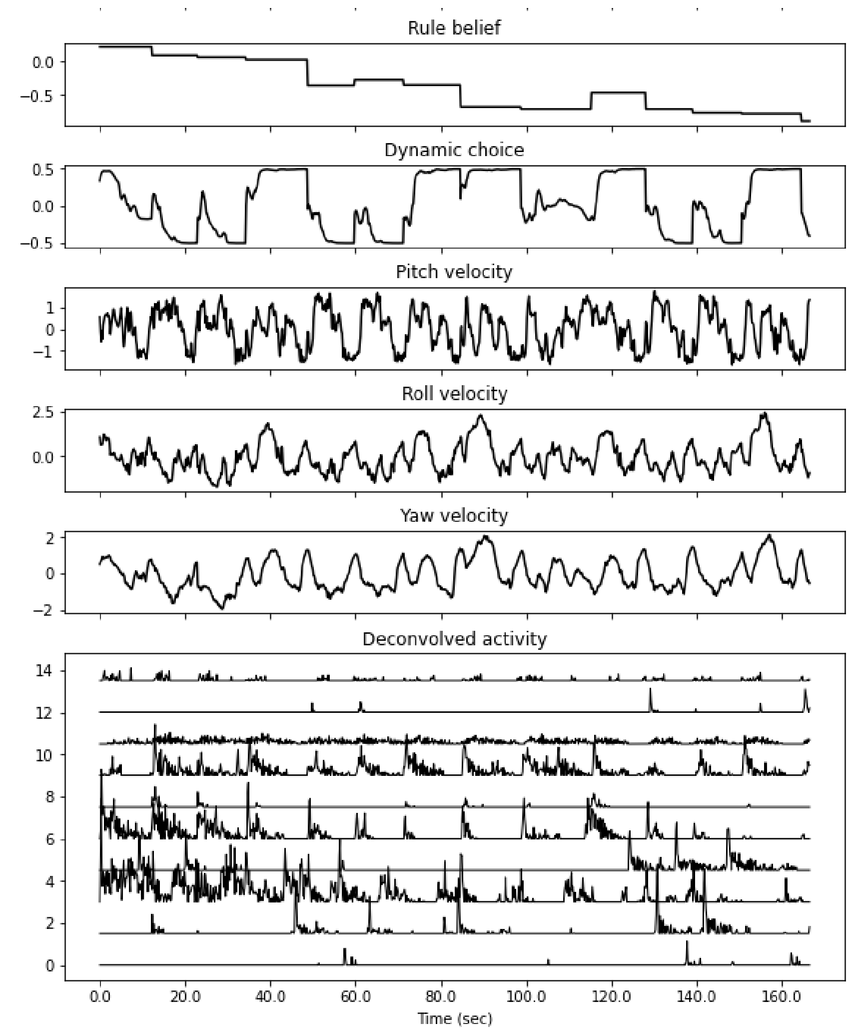
Tutorial_for_fitting_neural_calcium_imaging_data_with_GLM.ipynb
- Building design matrix (basis expansion)
- Model fitting, selection and evaluation
- Quantification of feature contribution



Tseng et al. 2022

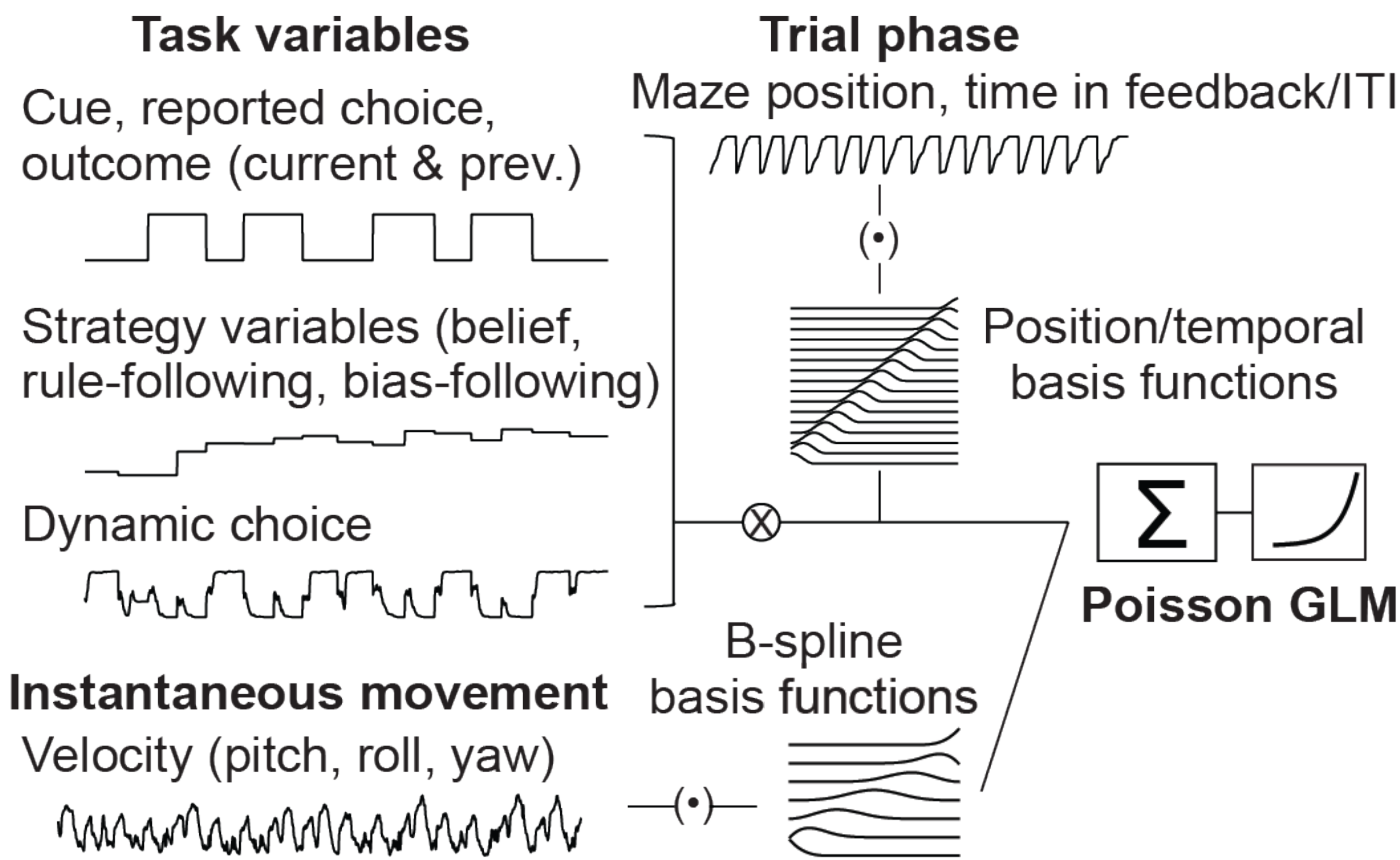
Predictors vs. neural activity





100 RSC neurons

Model schematic



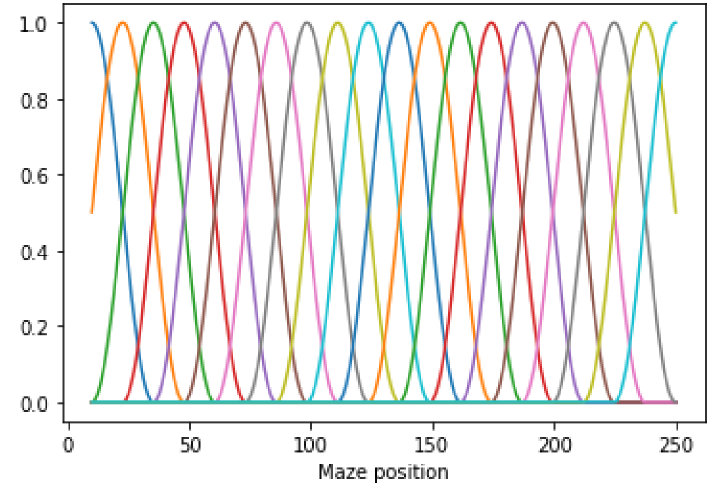
Position basis expansion

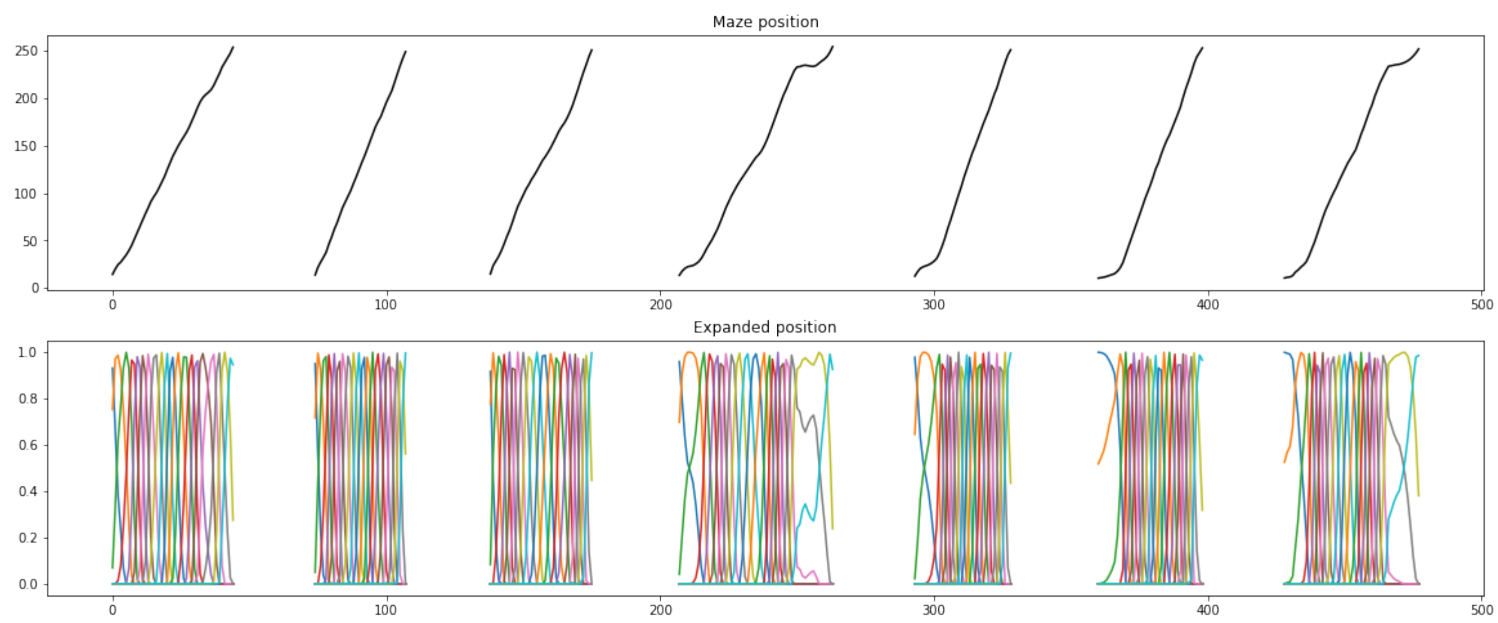
“Place field-like” tuning

Raised cosine bumps

$$f_i(x) = \begin{cases} \frac{1}{2}\cos(ax - \varphi_i) + \frac{1}{2} & \text{if } \varphi_i - \pi < ax \leq \varphi_i + \pi \\ 0 & \text{otherwise} \end{cases}$$

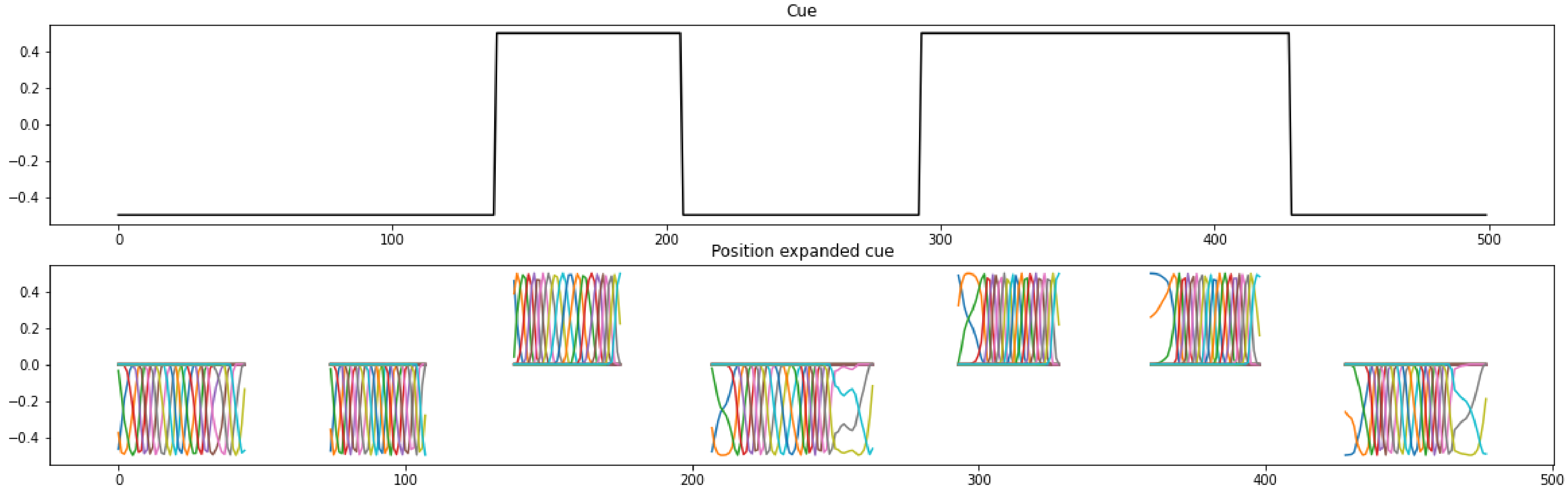
20 position bases spanning the maze





Load task variables onto position basis functions

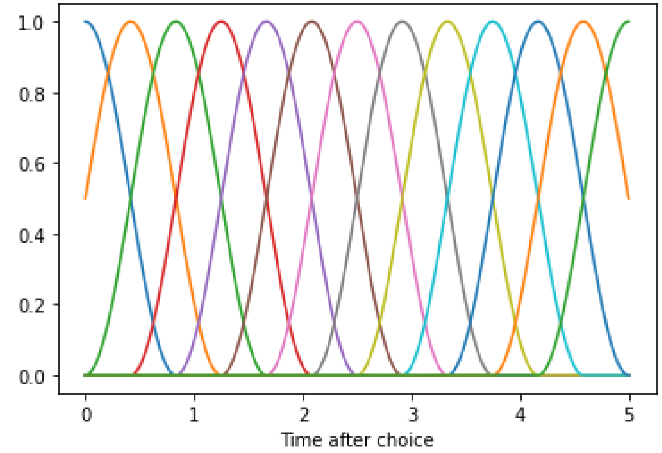
Simply take the **product** of the time series of task variables and each of the position basis functions, i.e. create **interaction terms**

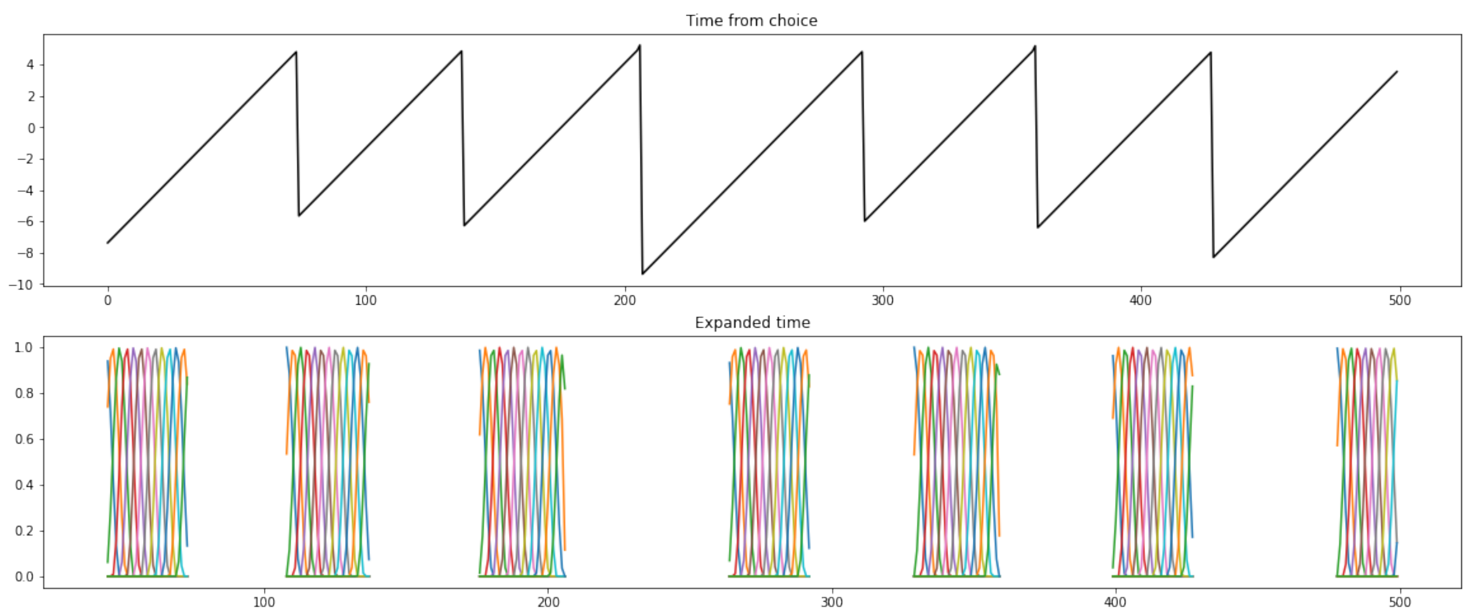


Temporal basis expansion

For time elapsed in feedback/ITI, follow the same principle to create temporal basis functions and load task variables onto them

13 temporal bases spanning feedback/ITI



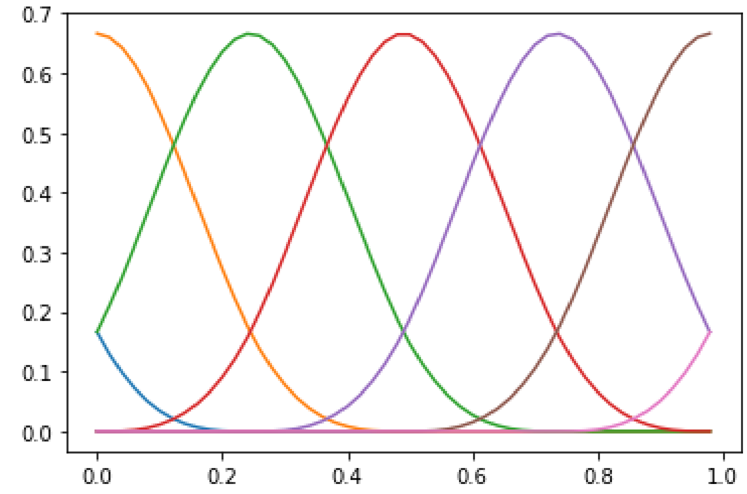


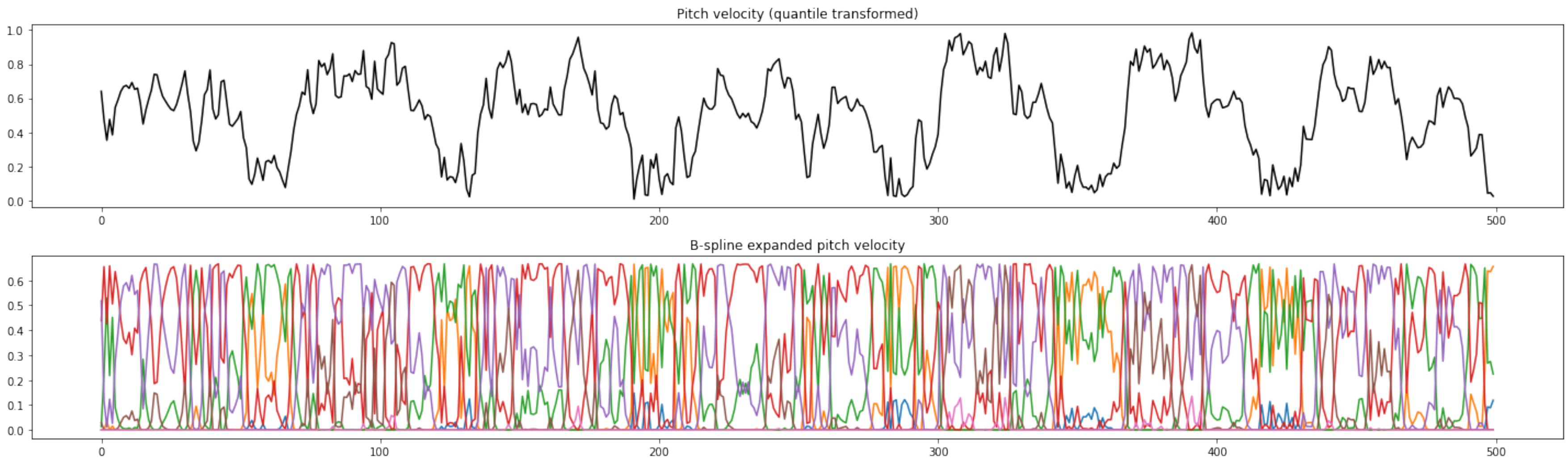
B-spline expansion for velocities

For movement variables, we assume *consistent relationship* btw neural activity and velocities (in maze vs. ITI)

Non-linear velocity tuning:
B-spline expansion (degree 3 polynomial)
Quantile transformation: easy comparison

7 b-splines spanning the quantile range

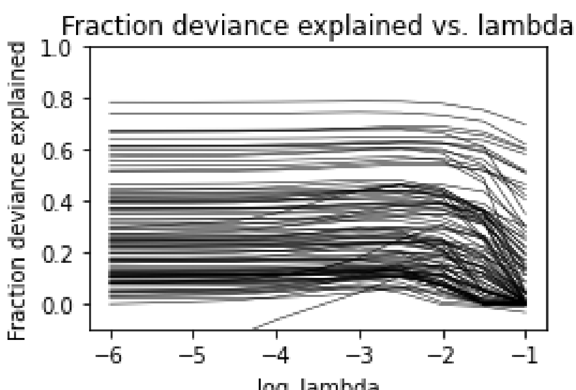


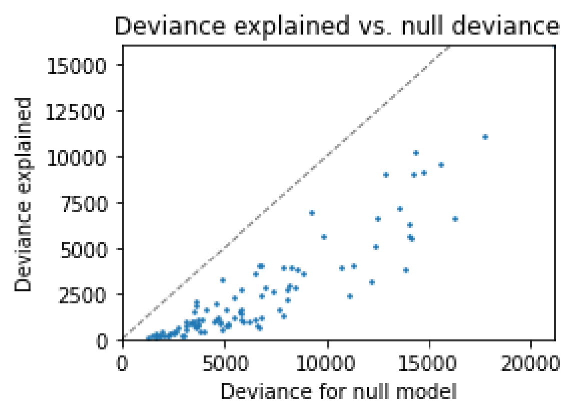


Fitting

- Poisson GLM, 5-fold cross validation
  - $Y = \exp(XW + W_0)$
  - Multiply deconvolved activity by 10 -> mimic spike count
- Regularization: group lasso
  - L2 for features belong to the same basis expanded groups
  - L1 between basis expanded groups
- Evaluation

$$\text{fraction deviance explained} = 1 - \frac{\text{model deviance}}{\text{null deviance}}$$



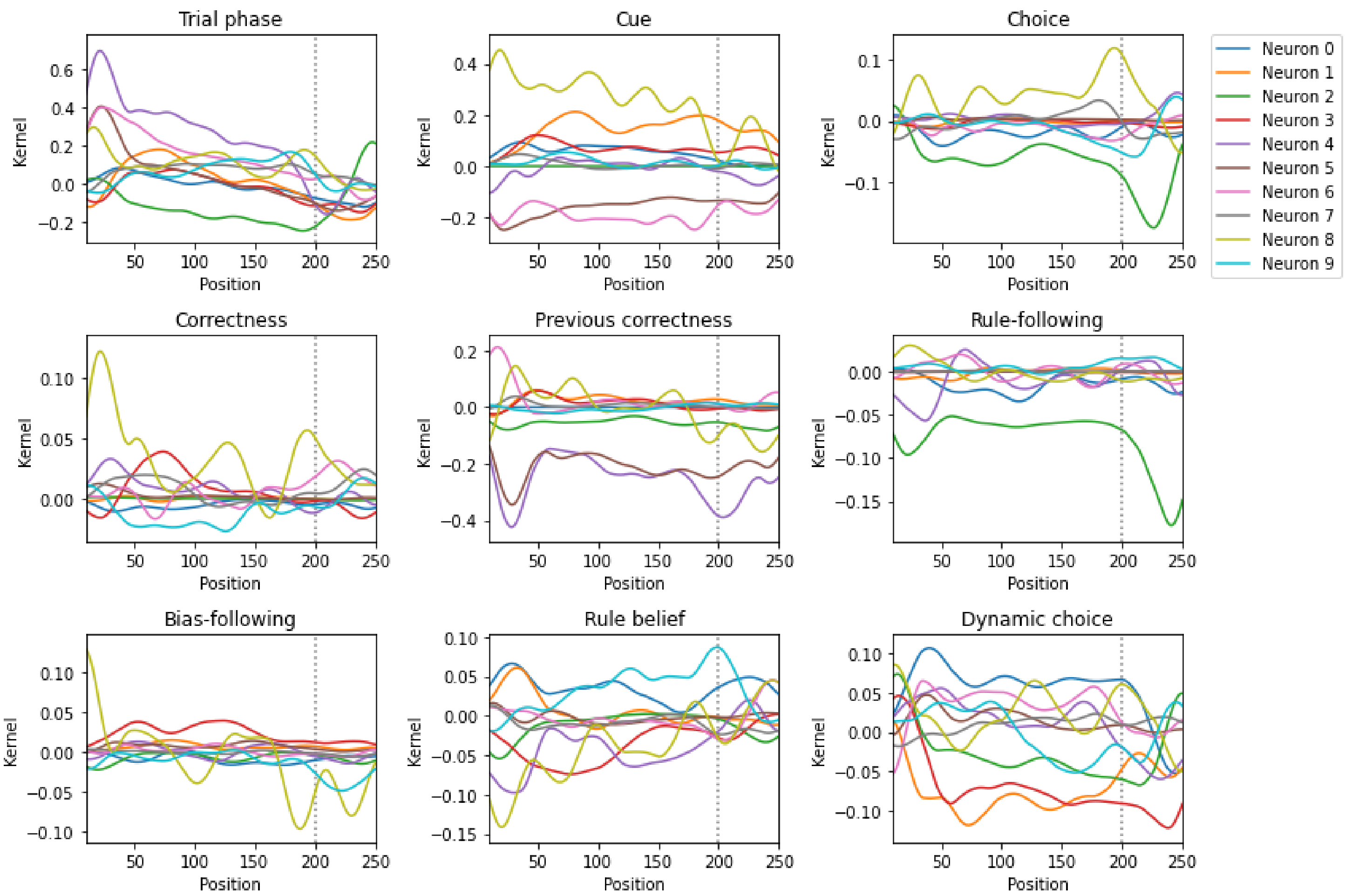


Quantification of feature contribution

- Model weights (kernels)
- Fraction null deviance or fraction explained deviance through model breakdown
- Fraction null deviance through model comparison with re-fitting

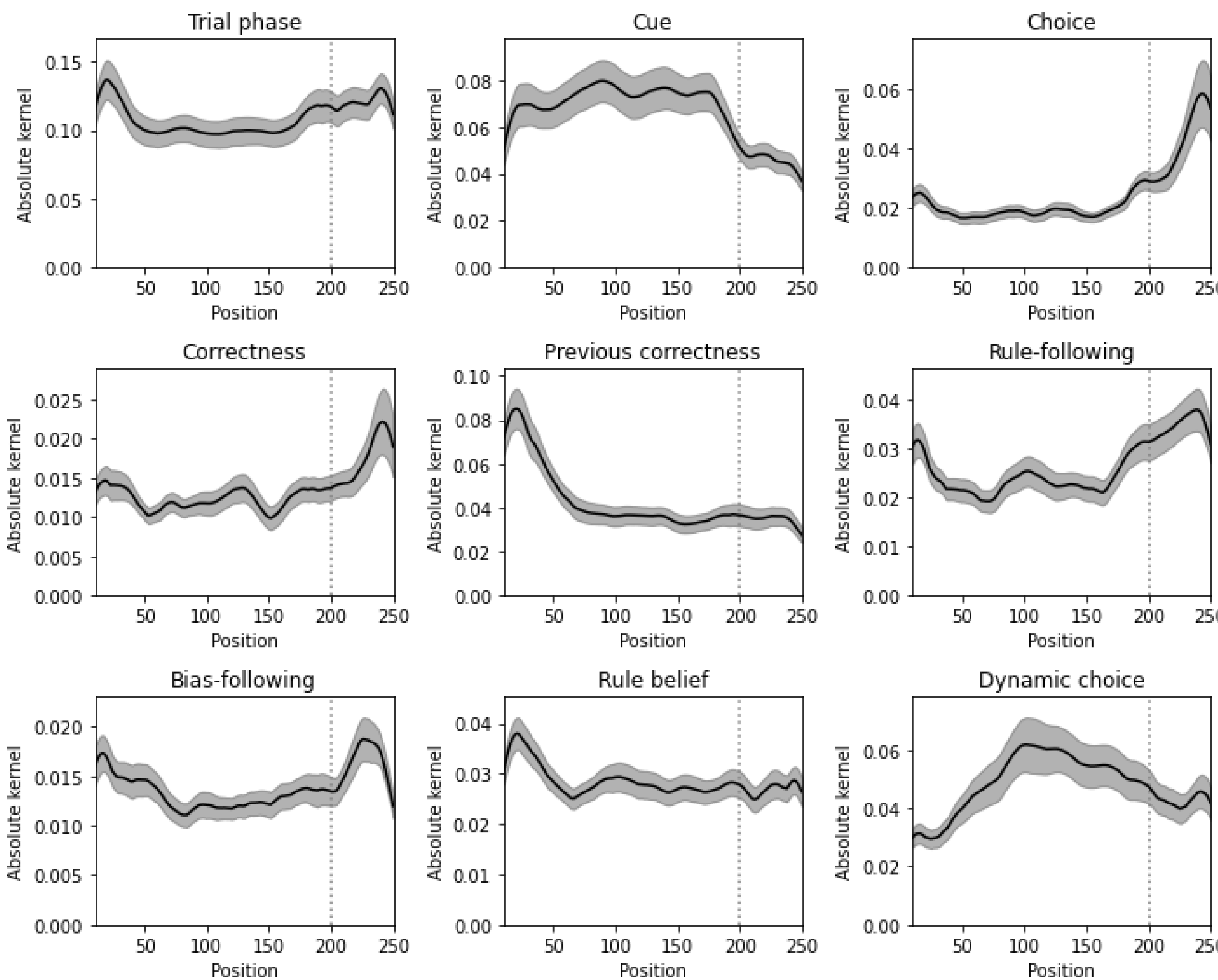
Model weights (kernels)

- Weight vector x basis functions -> sum up into kernels



Model weights (kernels)

- Mean absolute kernels: strength of tuning



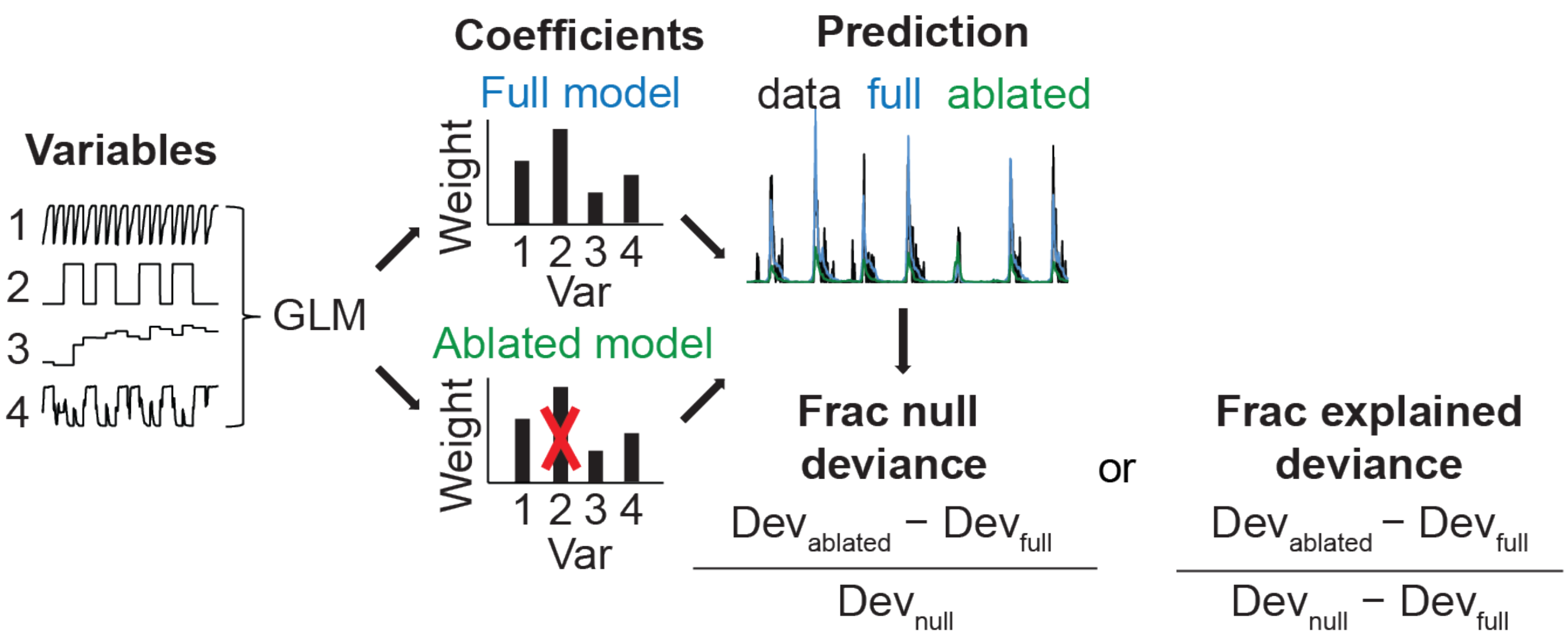
Model weights (kernels)

- Multiplicative factor on top of baseline activity
  - $y = \exp(w_0 + w_1x_1 + w_2x_2 + \ldots)$
  - Exponentiate to obtain "gain"
- Informative of directionality (signed)
- Robust to scaling of y
- Hard to interpret the magnitude and compare across variables
  - Better with "fraction null deviance" or "fraction explained deviance"

Model breakdown

"Model breakdown"

Quantification of variable contribution (without re-fitting)

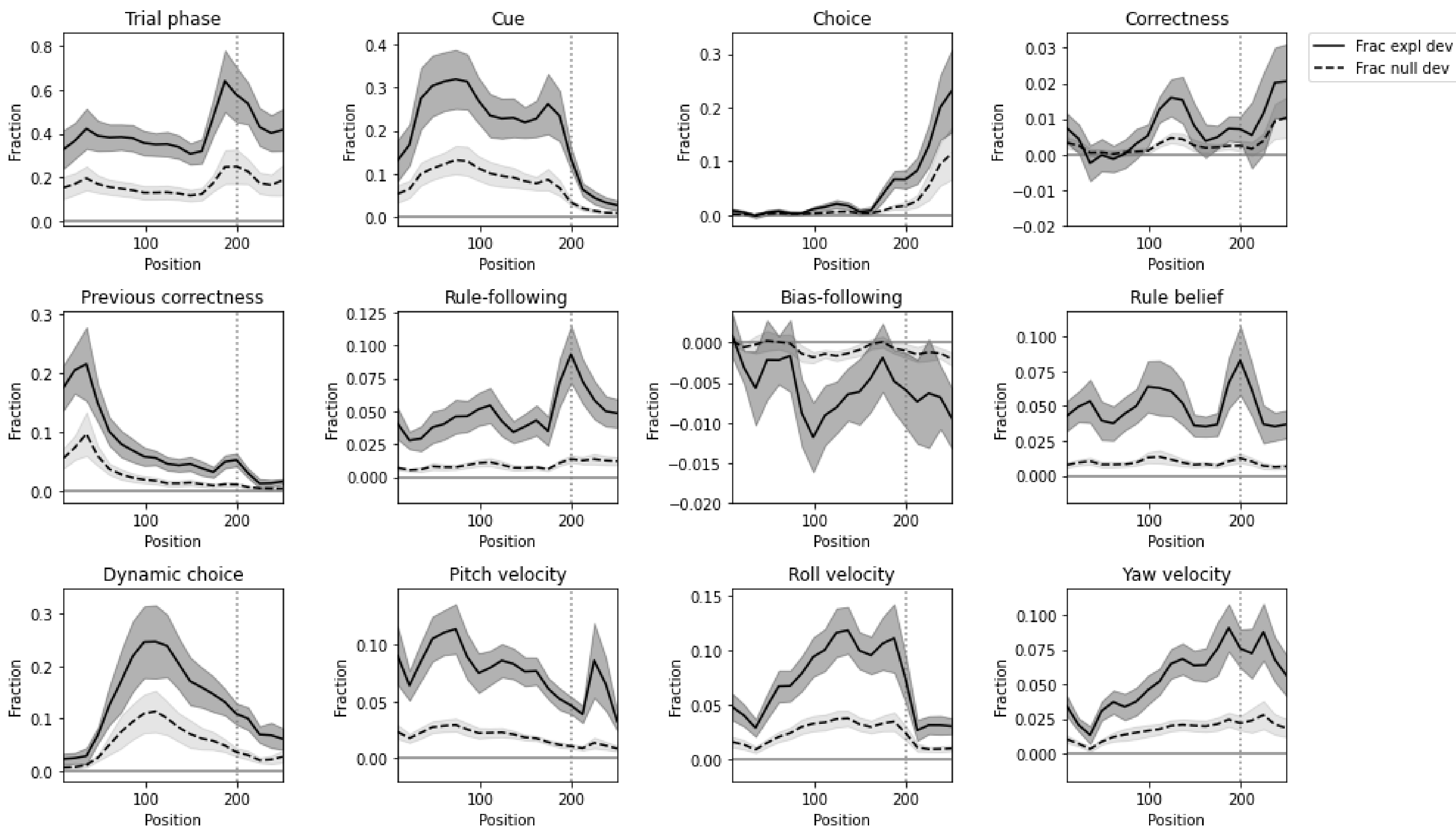


Zero weights = zero variables (must be zero-centered) = shuffle variables

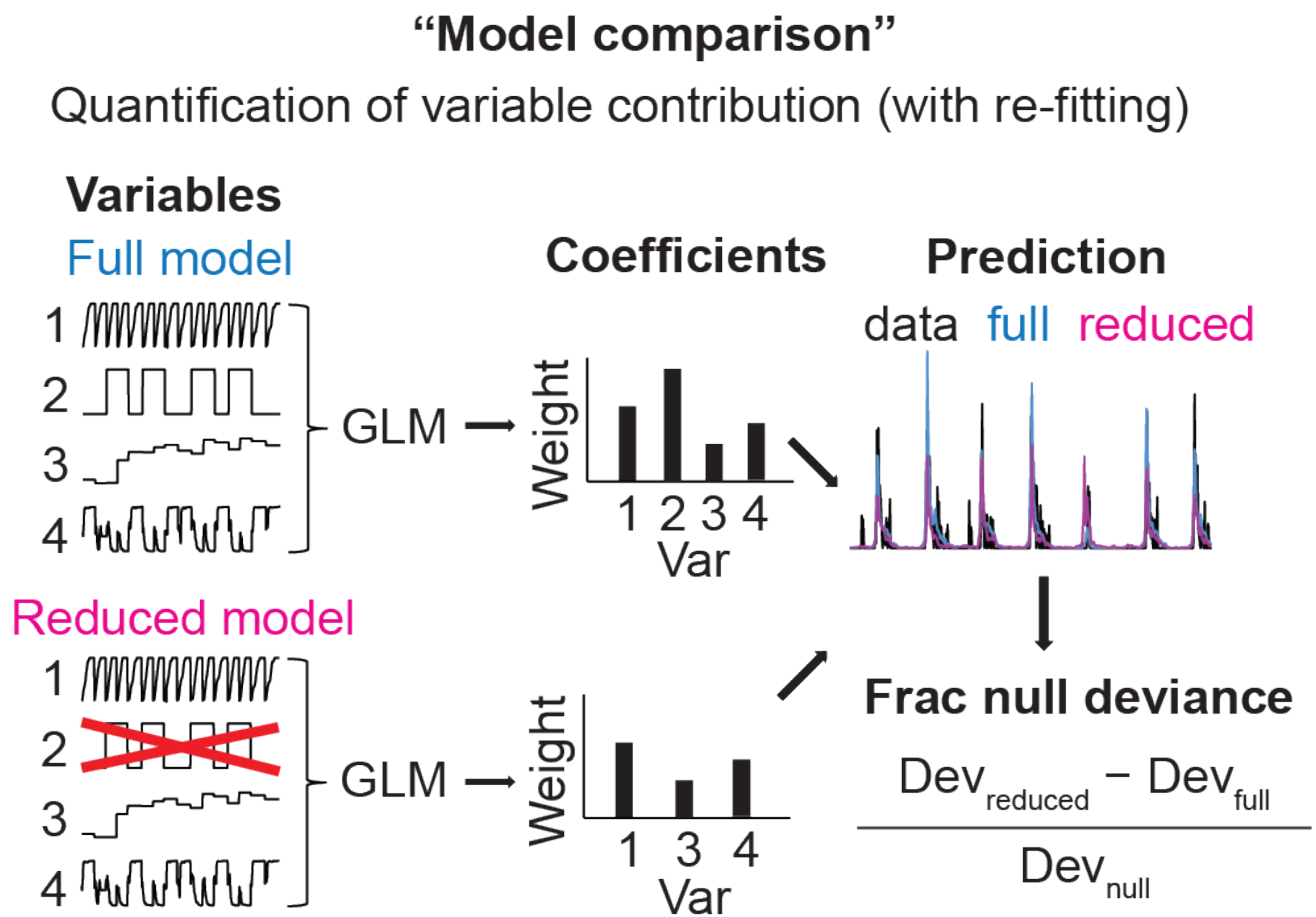
Evaluate on CV held-out data (85%) instead of test data (15%)

Model breakdown

Evaluate fraction null deviance or fraction explained deviance at each position (or time) bin



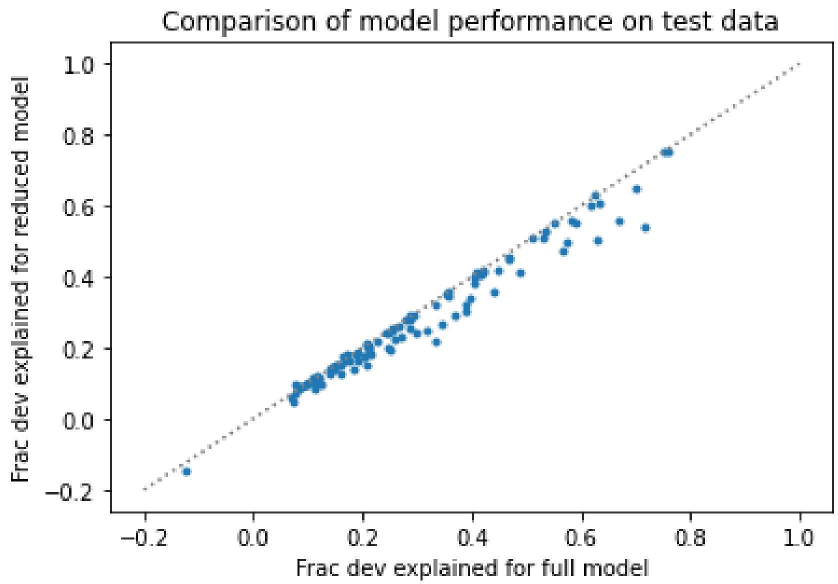
Model comparison (with re-fitting)

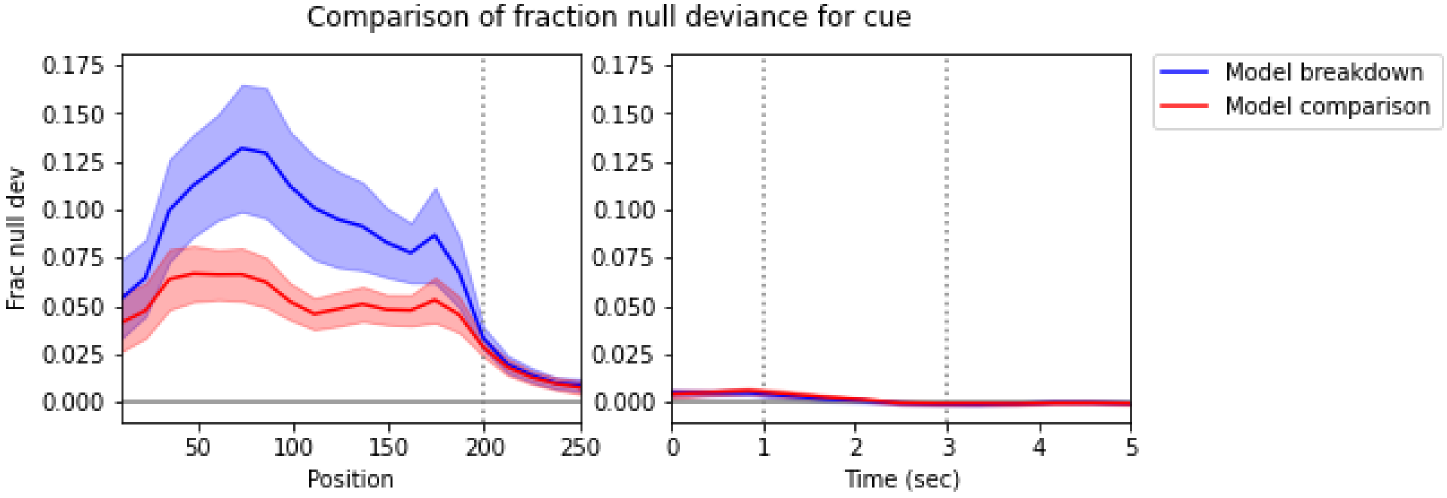


Remove variable = shuffle variable

Model comparison (with re-fitting)

For cue





Model comparison vs. breakdown

Model breakdown (fraction null deviance and fraction explained deviance)

- The metrics are easy to interpret and compare across variables
- Does not tell you the directionality of tuning
- Does not require re-fitting the model (fast to do)
- Not a linear breakdown for Poisson GLMs, but linear for Gaussian
- Can be less biased in assigning contribution of correlated variables, if the model is not terribly mis-specified

Model comparison (fraction null deviance)

- The metric is easy to interpret and compare across variables
- Does not tell you the directionality of tuning
- Require re-fitting of a model for each variable (computationally demanding)
- Extract the "unique" portion of deviance explained, can be biased (and underestimate the contribution of a variable) when there are correlated variables and you don't know which is actually contributing to response

References

- Tseng, S.-Y., Chettih, S.N., Arlt, C., Barroso-Luque, R., and Harvey, C.D. (2022). Shared and specialized coding across posterior cortical areas for dynamic navigation decisions. Neuron 110, 2484–2502.e16. [link]

- Minderer, M., Brown, K.D., and Harvey, C.D. (2019). The spatial structure of neural encoding in mouse posterior cortex during navigation. Neuron 102, 232–248.e11. [link]