- CV_M6_L01

Regression

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Regression

High-level problem definition:

- Supervised learning problem
- In general, inputs can be numerical or categorical data
  - For now, our focus is on numerical inputs
- Outputs are numerical

Regression

Error metrics

- Generally: a function of the difference between ground truth and predicted values
- Common:
  - Sum squared error (or mean squared error)
  - Sum absolute error (or mean absolute error)

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- Formulation of linear model
  - Scalar and vector formulations
  - With and without bias; incorporating bias term into input vector
- Graphical representation of the problem
- Error metrics
  - Mean squared error. rmse
  - Mean absolute error
- Solutions
  - Normal equation
  - Gradient descent

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Brain-Machine Interface Problem

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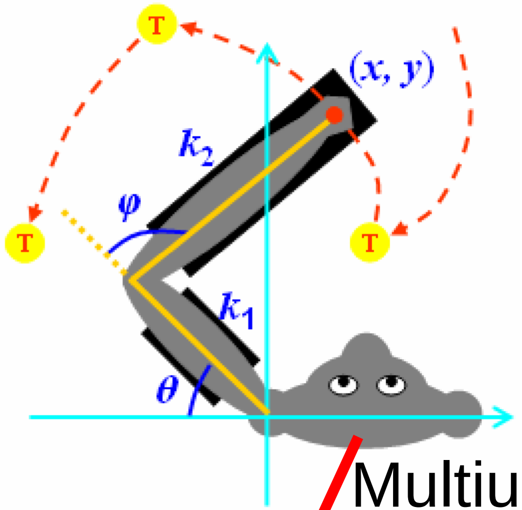
Brain-Machine Interfaces

Estimate of intended movement

Command prosthetic arm



Multiunit recording

Predictive model

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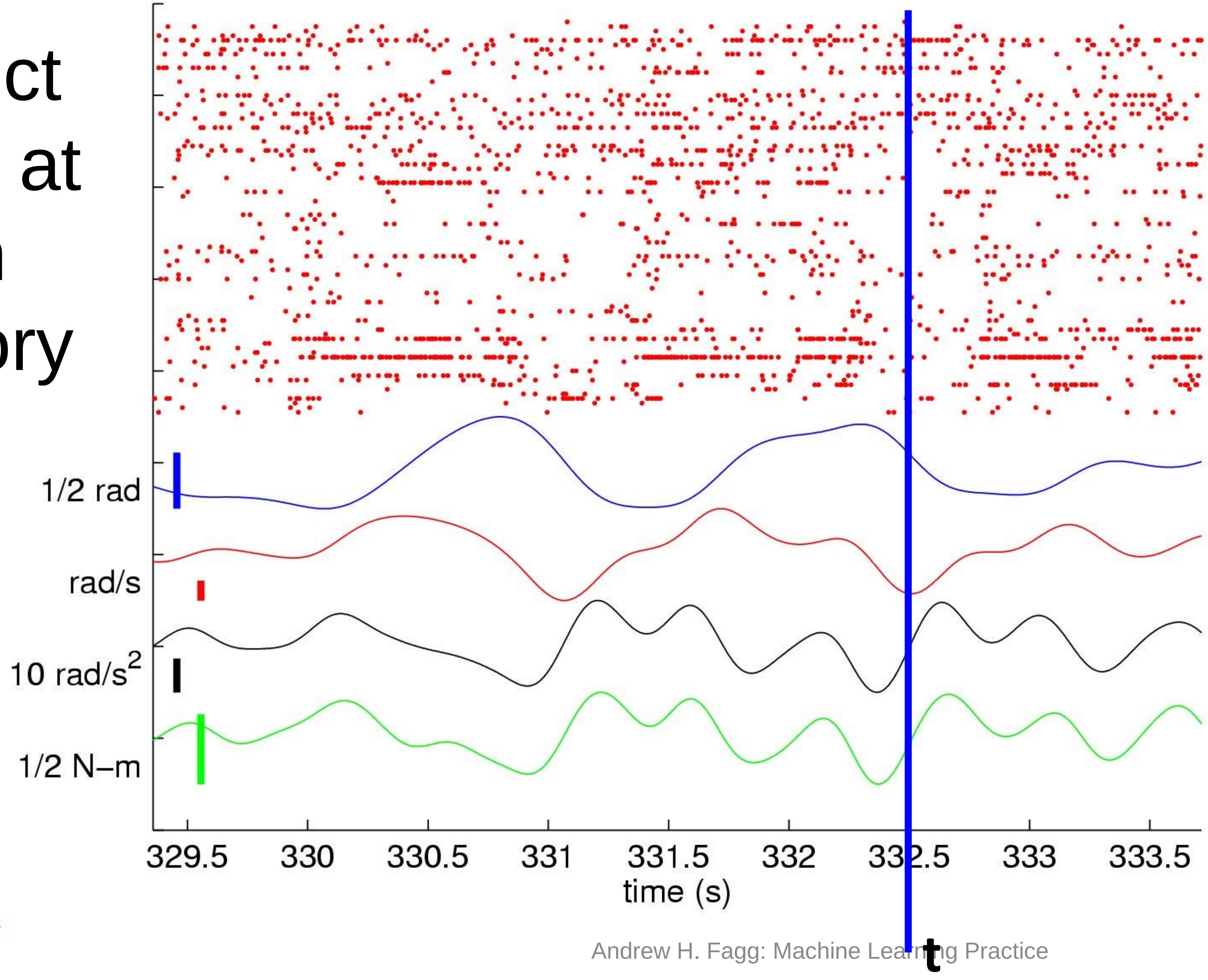
In collaboration with Nicholas G. Hatsopoulos and Lee E. Miller

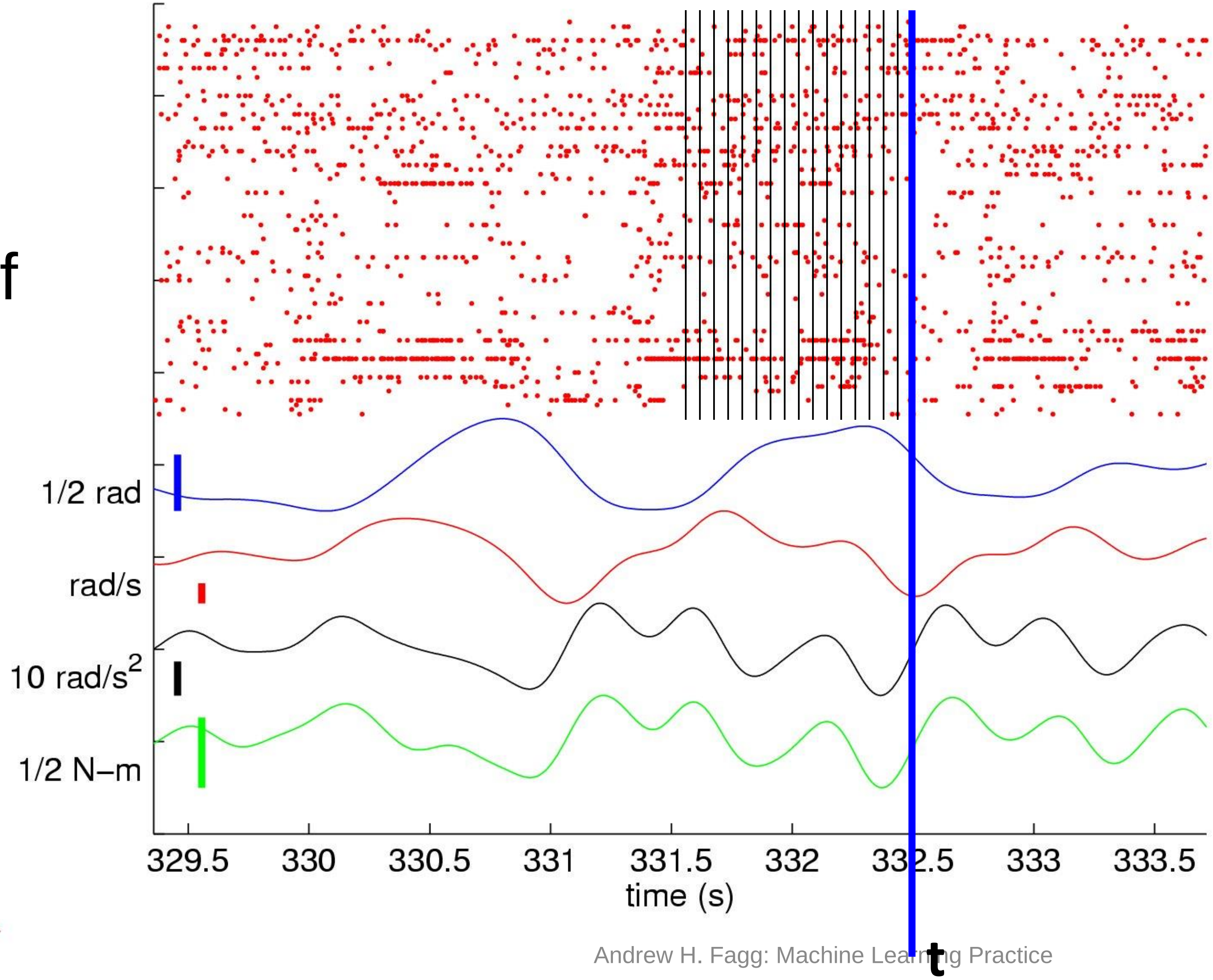
Decoding Arm State

Want to predict arm motion at time t given recent history of spiking behavior



Decoding Arm State

50ms bins: 20 descriptors of neural activation for each cell



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BMI Data Configuration

- Data already cut into 20 independent folds
- Time is continuous, but with gaps
  - We kept only valid time periods
- Each row in the CSV file contains 20 spike counts for each neuron
  - Each count corresponds to 50ms of time
  - A single row is a contiguous set of samples (no gaps!)

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Example: BMI Data

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Live demo

- Loading and organizing the BMI data

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Example: Predicting Arm Motion

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- LinearRegression example
  - Training set performance: plot and aggregate statistics
  - Test set performance

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Gradient Descent Methods

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Limits of the Normal Equation

- The "Normal Equation" requires the inversion of an N+1 x N+1 matrix, where N is the number of features
- This can be really expensive as N becomes large
  - And unnecessary if the features are rather sparse

Gradient Descent Methods

Gradient Descent Approach:

- Guess at an initial set of parameters
- Update the parameters in a direction so that the error metric is lowered
- Repeat until error is low enough or stops improving

Gradient Descent Challenges

- It is hard to tell *a priori* how many steps will be necessary
- Unclear what the "learning rate" should be
- Computing the gradient of the error with respect to the parameters:
  - Computation of the gradient is done for each training sample
  - These gradients are then summed together to estimate the global gradient
  - This is ***Batch Gradient Descent***
  - If the training set is large, then this is a computationally expensive process

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- Error surface
- Learning rate: too low to too high
- Different parts of the surface have different shapes
- Each sample "tugs on" the weights in some direction
  - Direction of movement in gd is the sum of these tugs
  - Want a way to estimate this sum without computing all of the tugs

Estimating the Gradient

- Stochastic Gradient Descent
  - Randomly select a single training example, compute the gradient and update the parameters
- Mini-Batch Gradient Descent
  - Cut the training set into batches
  - Use one batch at a time to compute gradient and update parameters
  - Cycle through these batches
- Stochastic Mini-Batch
  - Each training step: sample M training examples & use these to compute the gradient and update parameters

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Example: Gradient Descent Methods

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- Stochastic
- Batch
- Stochastic mini-batch

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Example: Training Sensitivity

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Number of Training Steps

How many training steps do we need for a given problem?

- This is an empirical question
- Can visualize using a learning curve
  - Take a small step
  - Record performance on a training set and a validation set
  - Repeat

Training Set Size

With our first regression-based models:

- Performance with the training set was high
- But, performance with an independent data set was generally quite poor
- In our problem, this is due to a dramatic over-fit of the training data
  - Note: 961 parameters and only 1193 samples

Training Set Size

Whenever we face a new problem, it is ***very important*** to ask the question of whether we have enough training data

- One approach: train a model with varying amounts of training data & ask how the model performs on an independent data set
- Sensitive to training set size: you are overfitting and need more data
- Insensitive: you have plenty of training data

Note that this is a model-specific (and hyper-parameter-specific) question

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Multi-Regression

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Multi-Regression

- So far, our models have only predicted a single output value for a given input
- In practice, we would like to handle entire vectors

Multi-Regression

Multi-regression is a generalization of regression

- Multiple outputs
- For our linear models, the parameters are completely separate from one-another
- Error metric is the sum of errors across the individual outputs

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- input / output pair notation
- Math behind the model
- Mean squared error:
  - Simple sum
  - Can be weighted sum

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Example: Multi-Regression

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- Predict two velocities

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Utility and Limits of Linear Regression

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Linear Regression

Utility:

- Inexpensive to evaluate models
- Can compute the solution to a problem directly ("Normal Equation")
- Gradient descent approach is straight-forward and relatively inexpensive computationally
- There is only one minimum in the error space

Linear Regression

Limits:

- The world is rarely linear
- Would like to capture non-linear effects
- Would also like to constrain the output to match our expectations of the valid range of outputs
  - For example, if we are trying to output a probability

Next Steps in Regression

- Non-linear preprocessing of input features
  - Otherwise, the model is linear
- Non-linear on the output of the model
  - Otherwise, the model is linear
  - Logistic regression
- Non-linearities built into the model throughout

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Non-Linear Preprocessing

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- General formulation: transformation of one vector to another
- Polynomial features
- Cosine features

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Example: Non-Linear Preprocessing

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- Polynomial transformation of the neural data

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The Overfitting Problem

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Overfitting

- Any situation where a model performs well on a training set, but not on an independent data set drawn from the same distribution as the training set
- In this case, the learned model has captured the peculiarities of the training set, but not the general trend of the entire distribution
- Detecting this situation is done by comparing model performance on training and independent data

Sources of Overfitting (or Apparent Overfitting)

- Training set is too small relative to the complexity of the model that is being fit
  - One clue: # of samples ~ # of model parameters
- Training set samples are not drawn independently
- Training data not actually drawn from the same distribution as the rest of the data

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- Overfitting polynomial example
- Example small random variation in an input dimension
  - Narrow Gaussian
  - Show a sampling that does not touch a tail
- LMS algorithm wants to fit a line with a very high slope
  - Show sample from tail
- Goal: want to limit the slopes
  - More generally: want functions that do not change rapidly

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Regularization

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Regularization

Approach: add terms to our cost function that punish models that have large coefficients

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- Linear model
- MSE
- Matrix math computation
- Ridge Regression
- Lasso
- Elastic Net

Regularization

- LMS: happy with high coefficients
- Ridge: wants to make coefficients small, especially ones that are already large
  - But, is happy to have very small coefficients
- Lasso: wants to make coefficients small
  - Wants to make as many coefficients zero as possible
- Elastic Net: also wants to make coefficients small
  - Can walk smoothly between the Ridge and Lasso solutions

Example: Regularization

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Example: Regularization

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Regularization

- Simple regression problem
- Compare Ridge, Lasso and Elastic Net Solutions

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Example: Regularization in the BMI Problem

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Example: Regularization in the BMI Problem

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Regularization in the BMI Problem

- We have already shown that LMS does not perform well with small training data set sizes
- How does regularization help with small training sets?

Example: Regularization in the BMI Problem

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