PHY604 Lecture 24

November 18, 2025

Today's lecture:
QMC and Neural networks

- Importance sampling in QMC

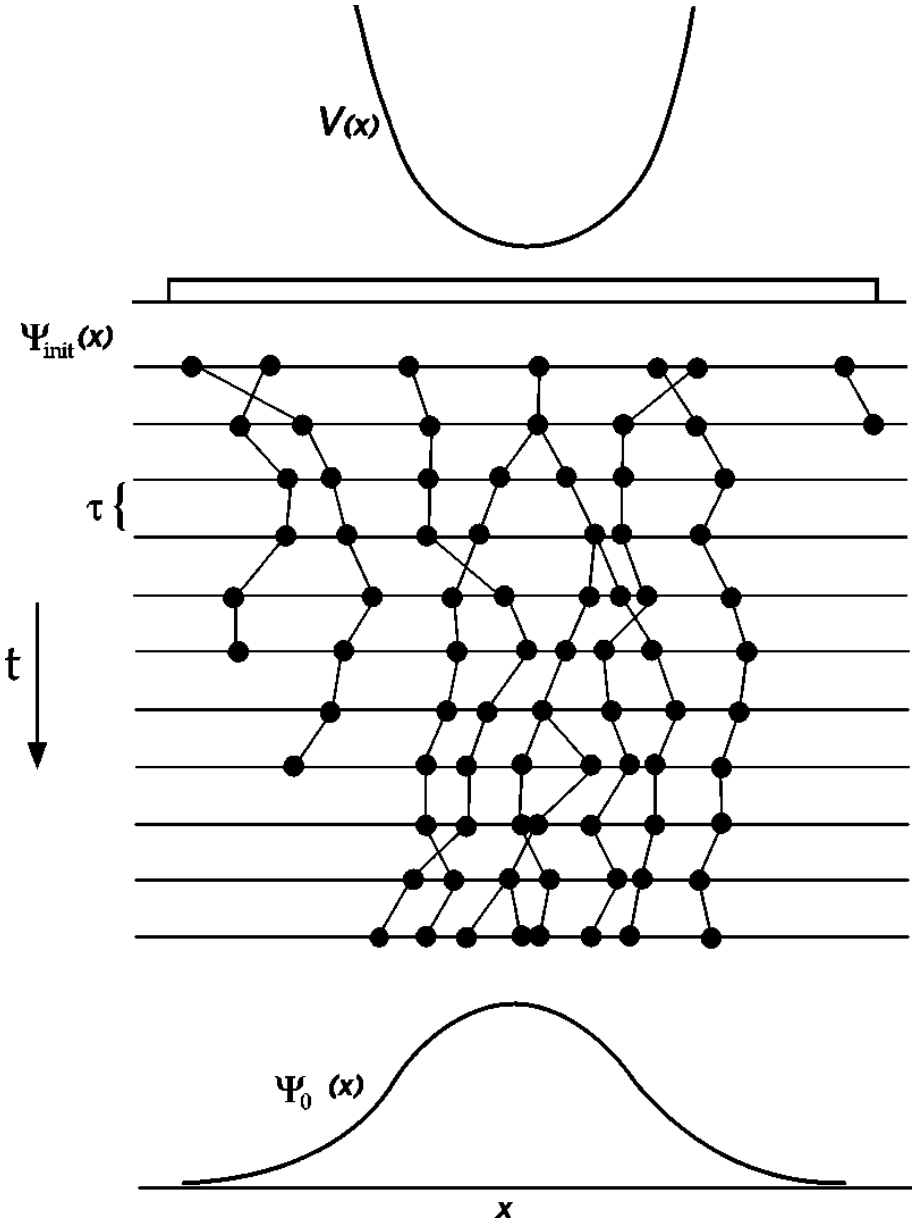
- Neural networks

Markov chain for QMC

- To do the Metropolis algorithm, we first create an ensemble of independent configurations: "random walkers"

- Propagate based on the diffusion part of Green's function G_d
  - As we showed, will propagate to ground state over time

- Use *P* as a "branching" probability distribution to choose whether:
  - Walker is killed
  - Walker continues its propagation
  - Walker continues its propagation and an additional one is spawned



Rev. Mod. Phys. 73 (2001)

Importance sampling in QMC

- Note that P exponentially suppresses propagation into high-potential areas, and potential may vary quickly and significantly
- We can make this more efficient with importance sampling
- Construct a "probability-like" function:

$$F(\mathbf{R}, t) = \Phi(\mathbf{R}, t)\Psi(\mathbf{R})$$

- Where Ψ is a trial wave function, e.g., from variational QMC
- This satisfies the diffusion equation:

$$\frac{\partial F}{\partial t} = \frac{1}{2}\nabla^2 F - \nabla \cdot F\mathbf{U} + [E_c - \mathcal{E}(\mathbf{R})]F$$

- Where we have a "drift" velocity: $U = \nabla \ln \Psi(\mathbf{R})$
- And we see again the local energy: $\mathcal{E}(\mathbf{R}) = \frac{1}{\Psi(\mathbf{R})} H\Psi(\mathbf{R})$

Modified Green's function

- Can show that the new Green's function is:

$$G(\mathbf{R},\mathbf{R}';\tau) \simeq (2\pi\tau)^{-3N/2} \exp\left[-\frac{[\mathbf{R}-\mathbf{R}'-\tau\mathbf{U}(\mathbf{R}')]^2}{2\tau}\right]$$
$$\times \exp\left[-\tau\frac{\mathcal{E}(\mathbf{R})+\mathcal{E}(\mathbf{R}')-2E_c}{2}\right]$$

- The drift velocity pushes random walkers towards areas of high density of the trial wave function

- If the trial wavefunction is good, the local energy is approximately constant, so second term does not vary too rapidly

Sign problem and fixed node approximation

- We have a crucial issue not yet discussed: Probabilistic methods like MC assume that probability distributions are positive
- Because we require wavefunctions of fermions to be antisymmetric, they cannot be positive everywhere
  - Need to assign a sign to the walkers, may change as they move through configuration space
- This leads to the fermion sign problem: If we sample over many configurations, we will get approximately zero
  - Gives decaying signal to noise ratio rather than the other way around

- Fixed node approximation: Take the zeros of trial wavefunction to be fixed and prevent walkers from changing sign

Importance sampling and the fixed node approximation

- Recall the Green's function we got from importance sampling:

$$G(\mathbf{R},\mathbf{R}';\tau) \simeq (2\pi\tau)^{-3N/2} \exp\left[-\frac{[\mathbf{R}-\mathbf{R}'-\tau\mathbf{U}(\mathbf{R}')]^2}{2\tau}\right]$$
$$\times \exp\left[-\tau\frac{\mathcal{E}(\mathbf{R})+\mathcal{E}(\mathbf{R}')-2E_c}{2}\right]$$

- Drift velocity carries walkers away from nodal surface
- Local energy also diverges near the nodal surface
- So, this importance sampling helps enforce the fixed node approximation
  - Walkers can still traverse a node if the time step is too big

One more issue: Approximation for Green's function poor near nodes

- Our approximation for the Green's function is not good when the drift velocity and local energy become large
- Could take smaller time steps to make sure we are pushed away from nodes
- Alternative approach: One more accept/reject step:
  - Accept propagation with probability:

$$w(\mathbf{R}', \mathbf{R}, \tau) = \frac{\Psi(\mathbf{R}')^2 G(\mathbf{R}', \mathbf{R}; \tau)}{\Psi(\mathbf{R})^2 G(\mathbf{R}, \mathbf{R}'; \tau)}$$

- This actually improves the approximation to the Green's function by enforcing a key property of the exact Green's function: detailed balance

Procedure for diffusion QMC

- 1. Perform a variational Monte Carlo simulation to optimize variational parameters in trial wave function.
- 2. Use the wavefunction from step 1 to generate an initial ensemble of configurations
- 3. Update with drift term and random walk χ: $\mathbf{R}' = \mathbf{R} + \mathbf{U}\tau + \chi$
- 4. Reject any step that crosses a node.
- 5. Accept the move with probability:

$$w(\mathbf{R}', \mathbf{R}, \tau) = \frac{\Psi(\mathbf{R}')^2 G(\mathbf{R}', \mathbf{R}; \tau)}{\Psi(\mathbf{R})^2 G(\mathbf{R}, \mathbf{R}'; \tau)}$$

- 6. Create a new ensemble of walkers using branching probability *P*
- 7. Measure local energy
- 8. Update E_c by averaging local energy over configurations **R** and **R'**

Some comments on QMC

- Quantum Monte Carlo is often the standard for accuracy for numerical calculations of solids and molecules

- It is at the basis of many other methods in condensed-matter physics
  - I.e., density-functional theory approximations rely on QMC of homogeneous electron gas
  - Solvers for embedding methods such as dynamical mean-field theory use ”continuous time” QMC

- The key to an efficient accurate scheme is how to deal with the sign problem

Machine learning

- Machine learning (ML) is the study of computer algorithms that can improve automatically through experience and by the use of data (Wikipedia)

- ML is a huge subject and is being applied in a wide range of scientific fields
  - Supervised learning: We know the “output” for some set of input data, want to know the output for the rest
  - Unsupervised: Take a set of inputs and find some structure
  - …

- We will focus our discussion: Supervised learning with neural networks

Patter recognition with computers

- Classic problem: Identify pictures of dogs versus cats
  - Easy for human, difficult for computer

Neural networks

- Neural networks attempt to mimic the action of neurons in a brain

- Good for problems where we have an incomplete or unsophisticated physical model, but a lot of data
  - Create a nonlinear fitting routine with free parameters
  - Train the network on data with known input and output to set the parameters
  - Trained network can be used on new inputs to predict outcome

- Help with pattern recognition, which is difficult for computers (often easy for humans)
  - Classic problem, identifying pictures of cats versus dogs

- Some uses:
  - Character / image recognition
  - AI for games
  - Classification of data
  - Finance

A simple linear model

- Represent input data as a vector *x*
- Represent output data as a vector *z*

- Simplest “model” that relates *x* and *z* is an unknown matrix **A**:

$$z = \mathbf{A}x$$

- This is just the same linear problem we have solved many times, but usually for *x* with a known **A**

- How can we get the values for **A**? If we have enough input/output data, we can figure it out

Solving for our linear model

- Say we have following data of input-output pairs:

$$x_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad z_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$x_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad z_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$x_3 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad z_3 = \begin{pmatrix} 4 \\ 1 \end{pmatrix}$$

- We want to find **A** such that:

$$z_1 = \mathbf{A}x_1, \quad z_2 = \mathbf{A}x_2, \quad z_3 = \mathbf{A}x_3,$$

Solving our linear model

- We write: $\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$
- Take the first two pairs: $\mathbf{A}x_1 = \begin{pmatrix} a \\ c \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\mathbf{A}x_2 = \begin{pmatrix} b \\ d \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

- Now **A** is fully specified: $\mathbf{A} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$
- But we can't fulfill the last condition:

$$\mathbf{A}x_3 = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \neq \begin{pmatrix} 4 \\ 1 \end{pmatrix} = z_3$$

Nonlinear models

- We saw with the previous example:
  - We can “train” a model using known inputs and outputs
  - A linear model is too “definite,” which is too restrictive
- Let’s run our linear model through a nonlinear function g(*x*):

$$g(x) = \begin{pmatrix} g(x_1) \\ g(x_2) \\ \vdots \\ g(x_n) \end{pmatrix}$$

- To get: $z = g(\mathbf{A}x)$

Nonlinear models

- Consider the simple nonlinear function: $g(p) = p^2$

- Solving the nonlinear equation with our inputs:

$$z_1 = g(\mathbf{A}x_1), \quad z_2 = g(\mathbf{A}x_2), \quad z_3 = g(\mathbf{A}x_3),$$

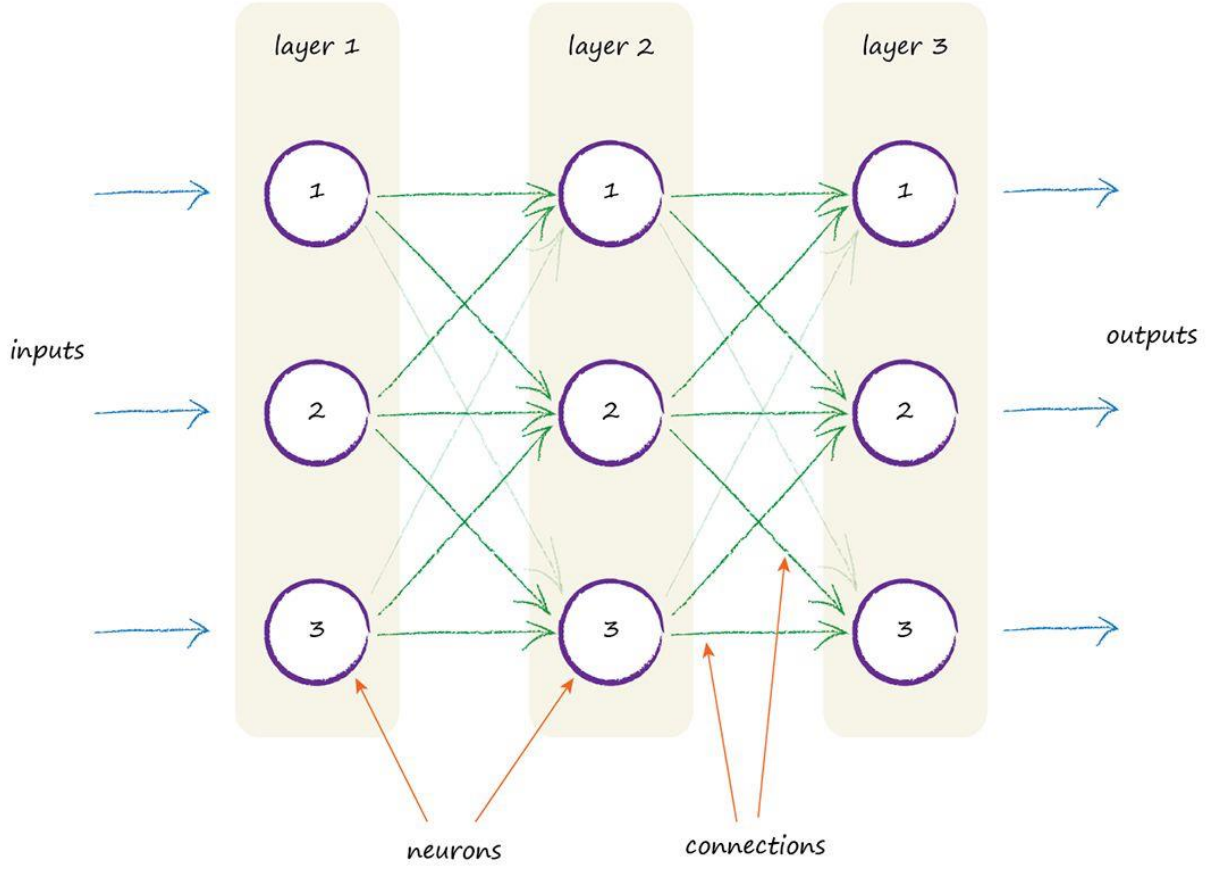
- Gives four valid solutions:

$$\mathbf{A}_1 = \begin{pmatrix} -1 & -1 \\ 0 & -1 \end{pmatrix}, \quad \mathbf{A}_2 = \begin{pmatrix} -1 & -1 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{A}_3 = \begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix}, \quad \mathbf{A}_4 = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

- Nonlinear models give much greater flexibility for describing data
- Tradeoff is that they are harder to solve

Nonlinear functions at the basis of neural networks

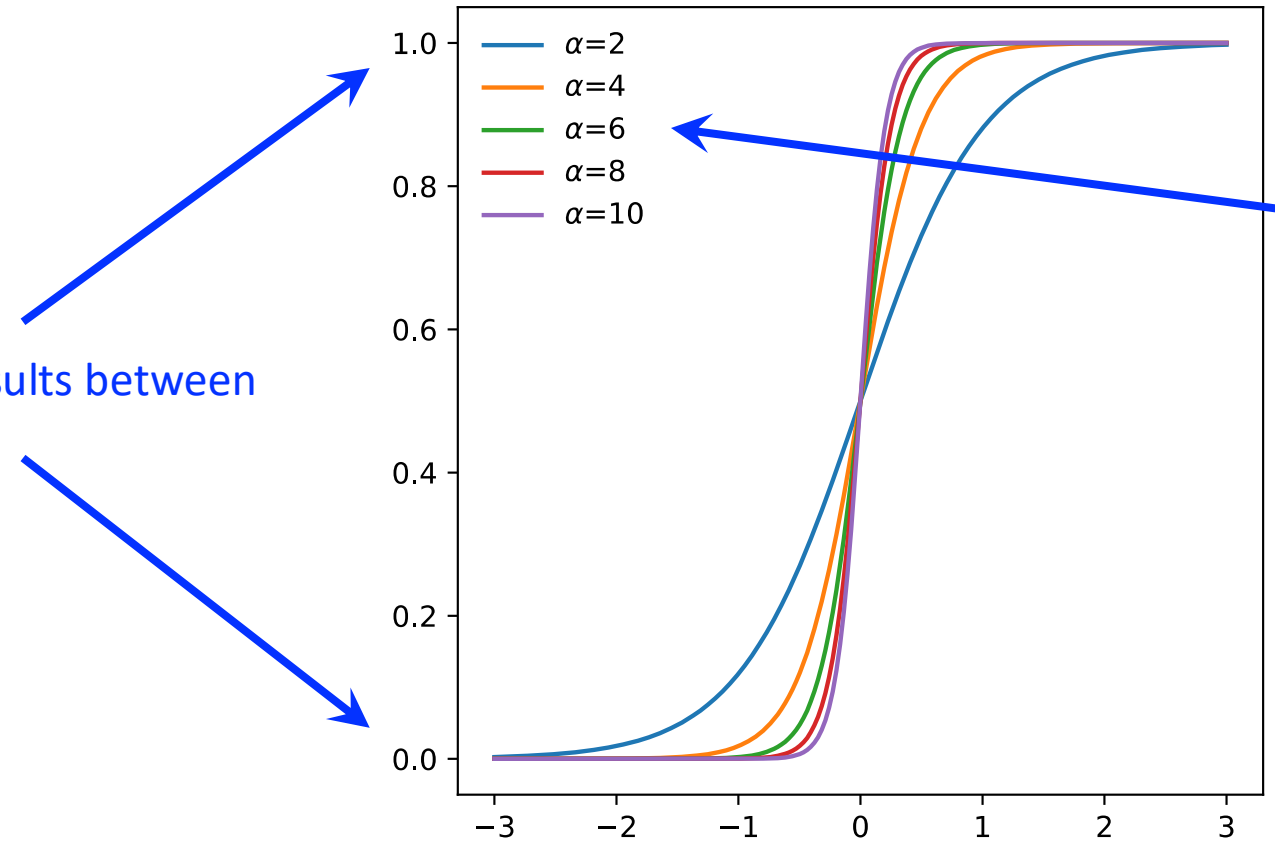
- Neural networks are divided into *layers*
  - Input layer accepts the input
  - Output layer outputs results
- Each layer has neurons (or nodes)
  - For input, one node for each input variable
  - Every node in the first layer connects to every node in the next layer
- Weight associated with the connection can be adjusted
  - These are the matrix elements
- Operations at neurons given by nonlinear activation function



Make Your Own Neural Network, Tariq Rashid

The sigmoid function for the nonlinear model

- What do we want from the nonlinear function?
  - For simplicity we will require that outputs are in the range (0,1)
  - We will need a function that is continuous and differentiable



Returns results between 0 and 1

α can be fixed or adjusted based on length of vectors

Neural network

- If we write the matrix-vector multiplication as:

$$(\mathbf{A}x)_i = \sum_{j=1}^{n} A_{ij}x_j$$

- Then the action of our neural network is:

$$z_i = g[(\mathbf{A}x)_i] = g\left[\sum_{j=1}^{n} A_{ij}x_j\right]$$

- Would like the elements of **A***x* to run over the nonlinear range of the sigmoid function. Choose for α:

$$\alpha = \frac{10}{n \ \max|x_i|}$$

Training our neural network

- Now we need to find the coefficients A_{ij}
- Assume we have some "training data" inputs *x* and outputs *y*

- Start with random entries in **A** in the range [-1,1]
- Minimize the difference between $g(\mathbf{A}x_j)$ and z_j
  - Function to be minimized:

$$f(A_{ij}) = |g(\mathbf{A}x_j) - z_j|^2$$

- We will minimize this function with the steepest descent method (see Lecture 12), iteratively update entries in **A** according to:

$$A_{ij} = A_{ij} - \eta \frac{\partial f}{\partial A_{ij}}$$

Gradient of minimization function

- Writing out the function explicitly:

$$f(A_{ij}) = \sum_{i=1}^{m} \left[g\left(\sum_{j=1}^{n} A_{ij} x_j \right) - y_i \right]^2$$

- Define:

$$b_i \equiv \sum_{j=1}^{n} A_{ij} x_j, \quad z_i \equiv g(b_i)$$

- Then:

$$f(A_{ij}) = \sum_{i=1}^{m} (z_i - y_i)^2$$

- And:

$$\frac{\partial f}{\partial A_{pq}} = \sum_{i=1}^{m} 2(z_i - y_i) \frac{\partial z_i}{\partial A_{pq}}$$

Gradient of minimization function

$$\frac{\partial f}{\partial A_{pq}} = \sum_{i=1}^{m} 2(z_i - y_i) \frac{\partial z_i}{\partial A_{pq}}$$

- Where:

$$\frac{\partial z_i}{\partial A_{pq}} = g'(b_i) \frac{\partial b_i}{\partial A_{pq}}$$

- And:

$$\frac{\partial b_i}{\partial A_{pq}} = \sum_{j=1}^{n} \frac{\partial A_{ij}}{\partial A_{pq}} x_j = \sum_{j=1}^{n} \delta_{ip} \delta_{jq} x_j = \delta_{ip} x_q$$

Gradient of minimization function

- Because of our form of *g*, we have:

$$g'(p) = \frac{\alpha e^{-\alpha p}}{(1+e^{-\alpha p})^2} = \alpha g(p)[1-g(p)]$$

- So:

$$\frac{\partial z_i}{\partial A_{pq}} = \alpha g(b_i)[1-g(b_i)]\delta_{ip}x_q = \alpha z_i(1-z_i)\delta_{ip}x_q$$

- And:

$$\frac{\partial f}{\partial A_{pq}} = \sum_{i=1}^{m} 2(z_i - y_i)\alpha z_i(1-z_i)\delta_{ip}x_q = 2\alpha(z_p - y_p)z_p(1-z_p)x_q$$

Comments on using the neural network

- Once we have trained **A**, then we can use our neural net on some input *w* for which we don't know the output by calculating $g(\mathbf{A}w)$
- Have to set a value of α prior to training (using the max of all of the input data)
- Note that once the matrix **A** has been adapted for a given input/output pair, it will generally not work anymore for the previous pairs. To get around this:
  - Generate *t* sets of input/output training data
  - Repeat the sets *Nt* times, and run them through at random

Procedure for doing “Machine Learning” with neural network

- 1. Choose a nonlinear activation function (in our case, find α)
- 2. Choose/generate *t* input/output pairs for training
- 3. Repeat the set from step 2 *N* times (epochs) to get a training set of *T*=*Nt* pairs
- 4. Run the training set through the neural net at random, performing the steepest descent minimization for each
- 5. To test the training in step 4, run the *t* examples through and calculate the residual:

$$g(\mathbf{A}x_j) - z_j$$

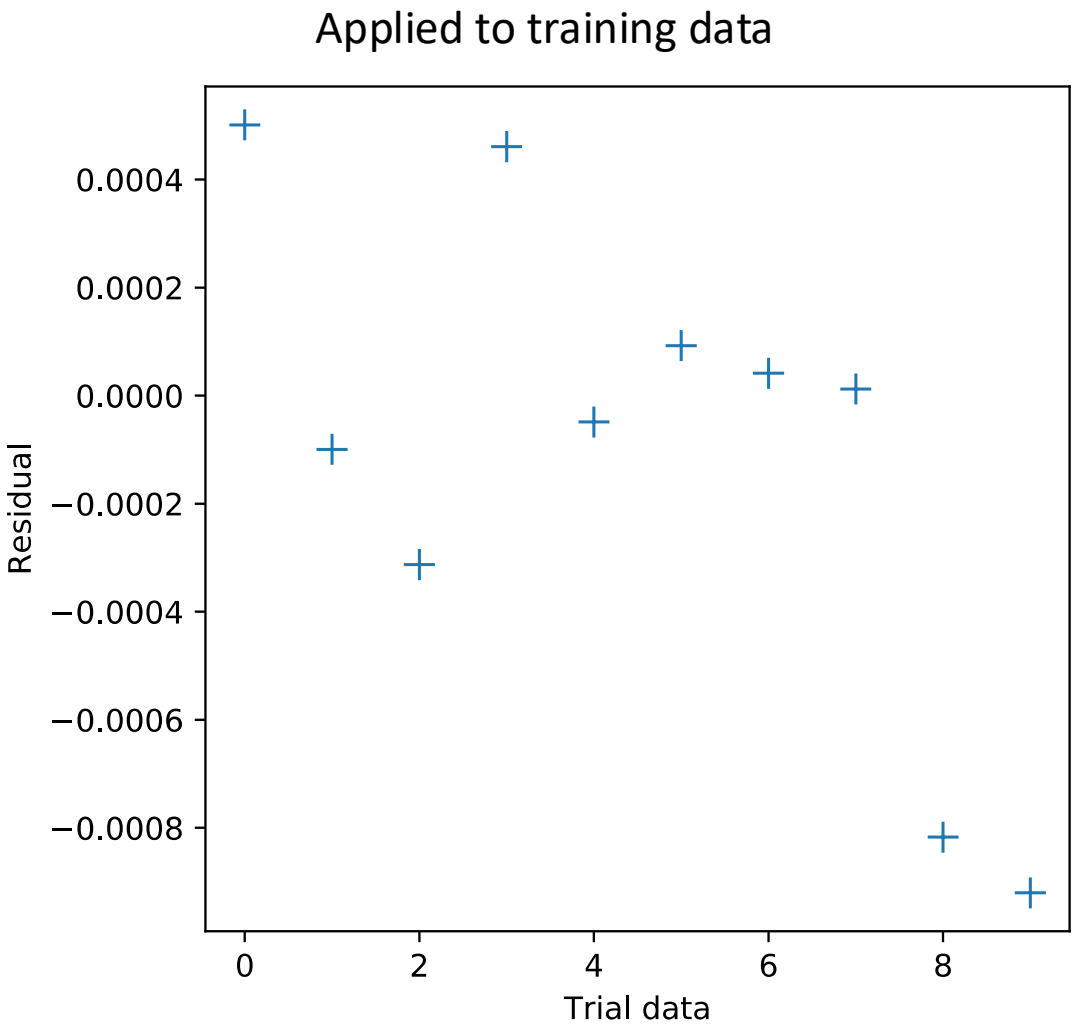
- 6. Use the neural net on some new data

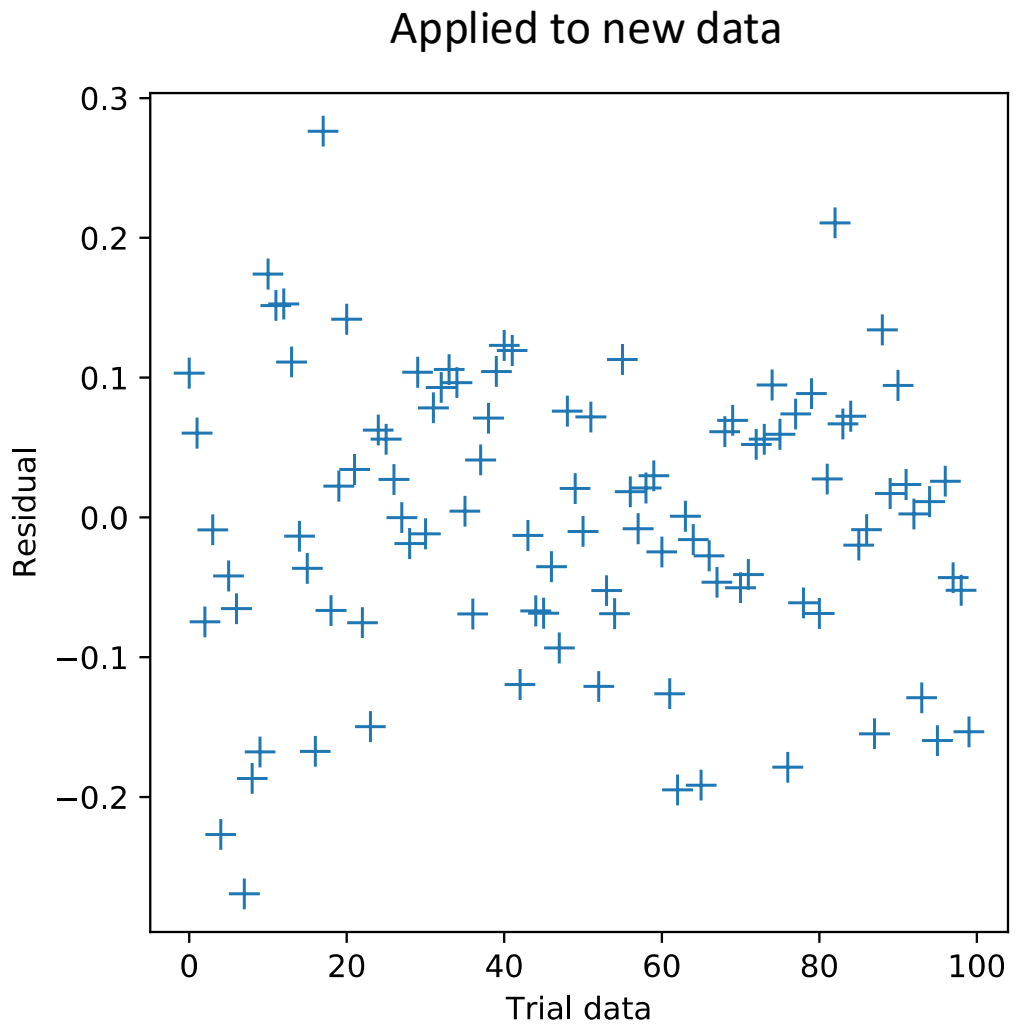
Simple example of a neural net

- Input data: Ten randomly chosen numbers from a set
- Output data: The tenth number in the set
- Make a training set of 10 input/output pairs
- Run it through randomly 100 times to train **A**
- Expect something like:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Results from our neural net





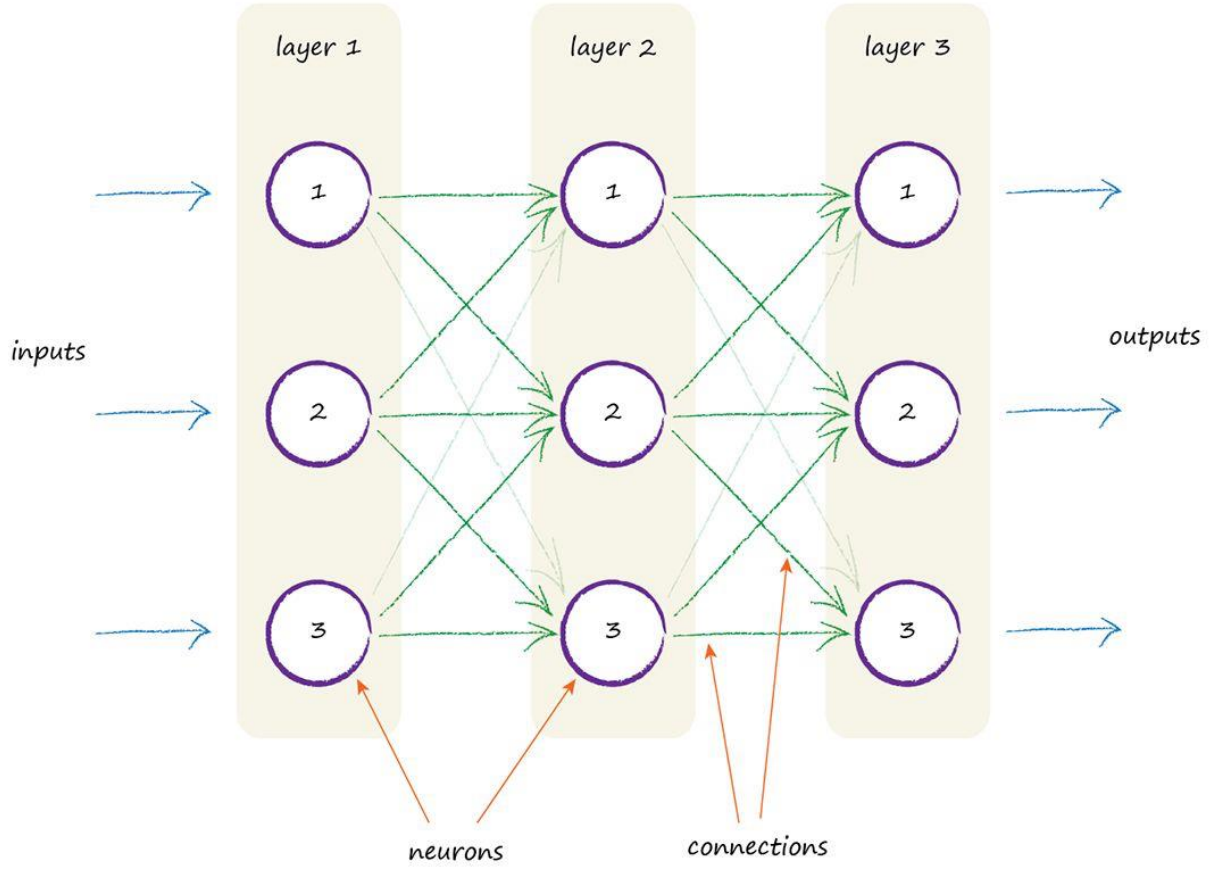
$$\mathbf{A} = \begin{bmatrix} -0.04 & 0.42 & 0.15 & -0.23 & 0.13 & 0.06 & 0.19 & -0.42 & 0.48 & 4.45 \end{bmatrix}$$

Adding additional degrees of freedom

- In the previous example, the number of adjustable parameters is constrained by the size of the input and output

- To overcome this limitation, we can add hidden layers to our neural net

- Will need an additional matrix and an additional evaluation of out nonlinear function



Make Your Own Neural Network, Tariq Rashid

Hidden layers

- Take as input a vector *x* of length *n*
- Take as input a vector *z* of length *m*
- Consider a *k* x *n* matrix **B** and a *m* x *k* matrix **A**
- Construct the output as:

$$\widetilde{z} = g(\mathbf{B}x) - \frac{1}{2}, \qquad z = \widetilde{g}(\mathbf{A}\widetilde{z})$$

- Note that we differentiate the applications of *g* because they may have different α's
- Extra shift of ½ is to recenter the data around 0 to put it in the nonlinear range of *g*
- Key: *k* is independent of the size of input/output!
  - Can train *k*(*m*+*n*) total elements

Implementing the hidden layer

- We still want to minimize our cost function *f*:

$$f(A_{rs}, B_{ij}) = \sum_{r=1}^{m} (z_r - y_r)^2$$

- Now we have to do two interrelated steepest descent minimizations:

$$A_{pq} = A_{pq} - \eta \frac{\partial f}{\partial A_{pq}}, \qquad B_{pq} = B_{pq} - \eta \frac{\partial f}{\partial B_{pq}}$$

- Where:

$$\frac{\partial f}{\partial A_{pq}} = 2\widetilde{\alpha}(z_p - y_p) z_p (1 - z_p) \widetilde{z}_q \equiv \sigma_p \widetilde{z}_q$$

$$\frac{\partial f}{\partial B_{pq}} = \sum_{r=1}^{m} \sigma_r A_{rp} \alpha \left(\frac{1}{2} + \widetilde{z}_p\right) \left(\frac{1}{2} - \widetilde{z}_p\right) x_q$$

Back propagation

- Note that we are optimizing simultaneously **A** and **B**:

$$\frac{\partial f}{\partial A_{pq}} = 2\widetilde{\alpha}(z_p - y_p)z_p(1 - z_p)\widetilde{z}_q \equiv \sigma_p \widetilde{z}_q$$

$$\frac{\partial f}{\partial B_{pq}} = \sum_{r=1}^{m} \sigma_r A_{rp} \alpha \left(\frac{1}{2} + \widetilde{z}_p\right)\left(\frac{1}{2} - \widetilde{z}_p\right) x_q$$

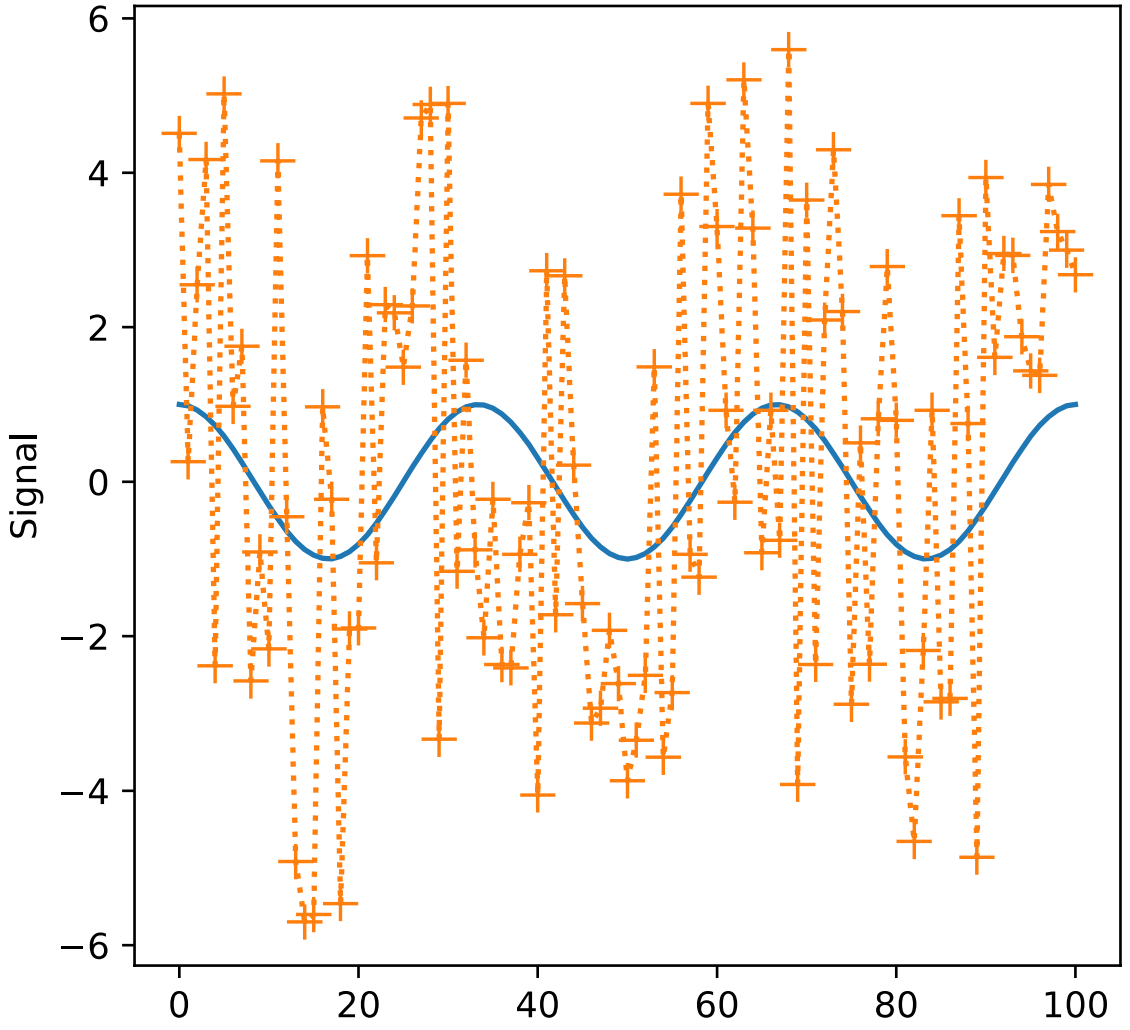
- So, the errors are “backpropagated” through the output and hidden layers

Example: Signal analysis

- Given a noisy signal expected to be one of four frequencies
  - f ={1,2,3,4} Hz
- Noise is significantly larger than the underlying signal:

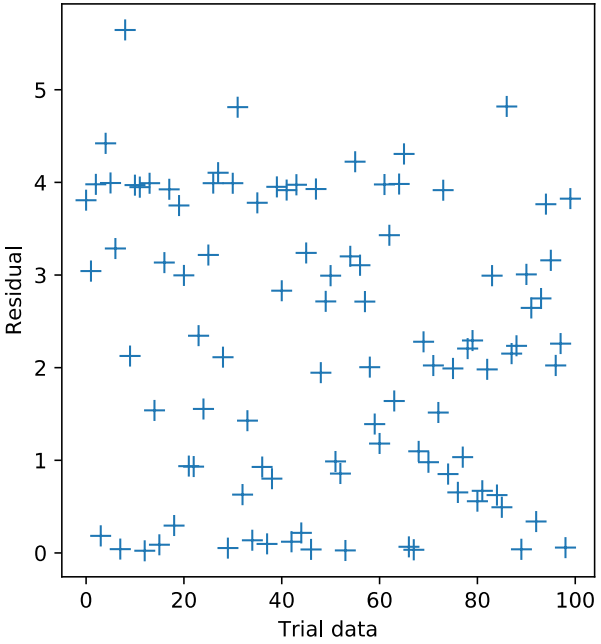
$$s(t) = \cos(2\pi f t) + 5\xi$$

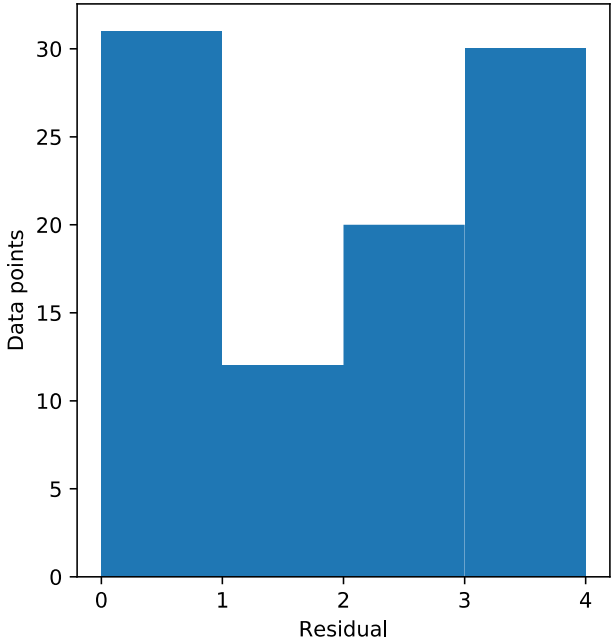
  - ξ is a random number in [-1,1]
- Can we identify the frequency?



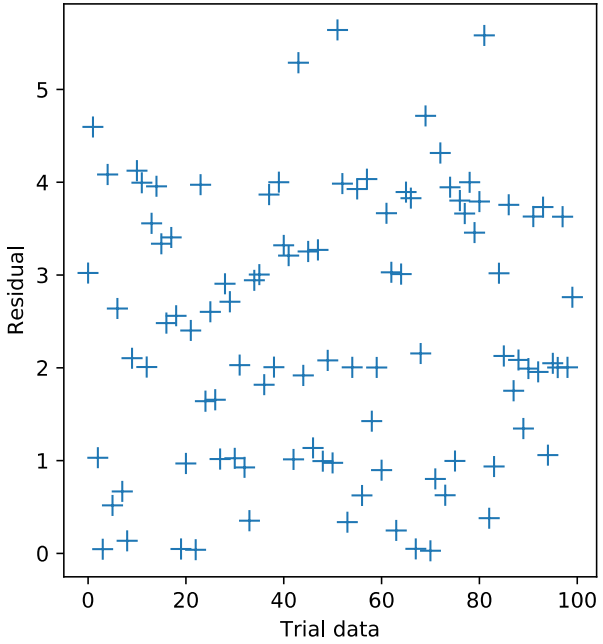
Signal analysis: Hidden layers size 2

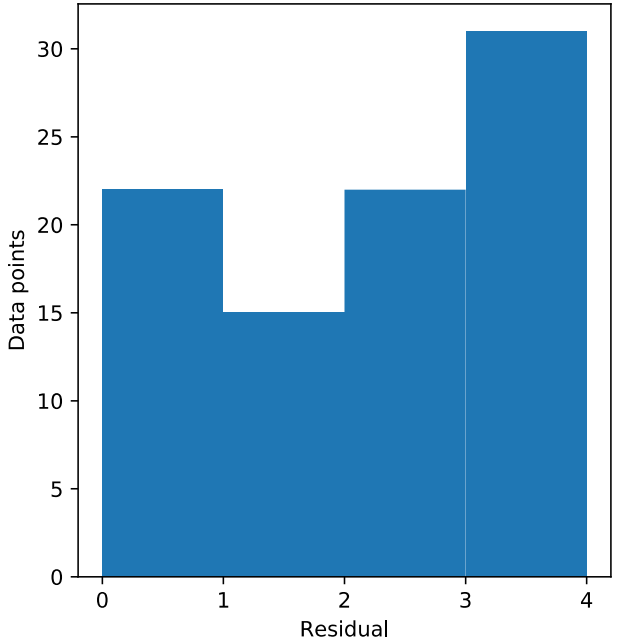
Test on the training set





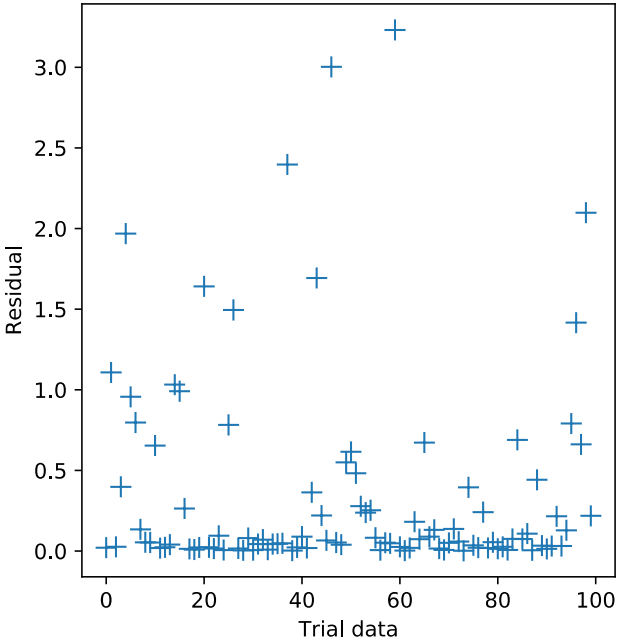
Test on new data

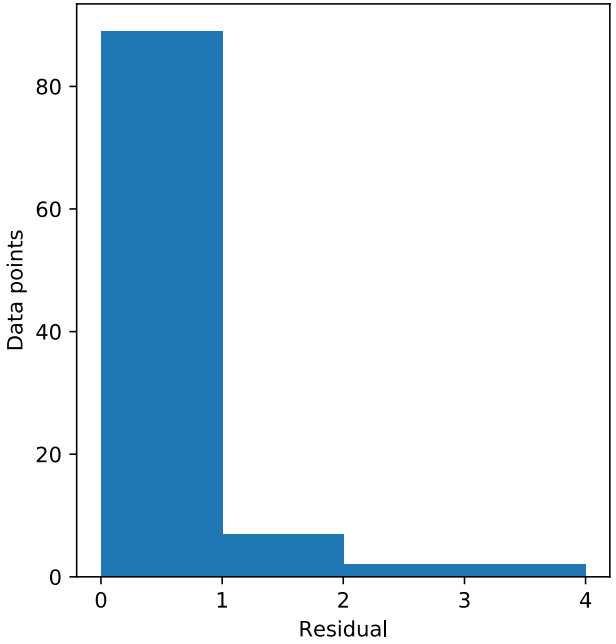




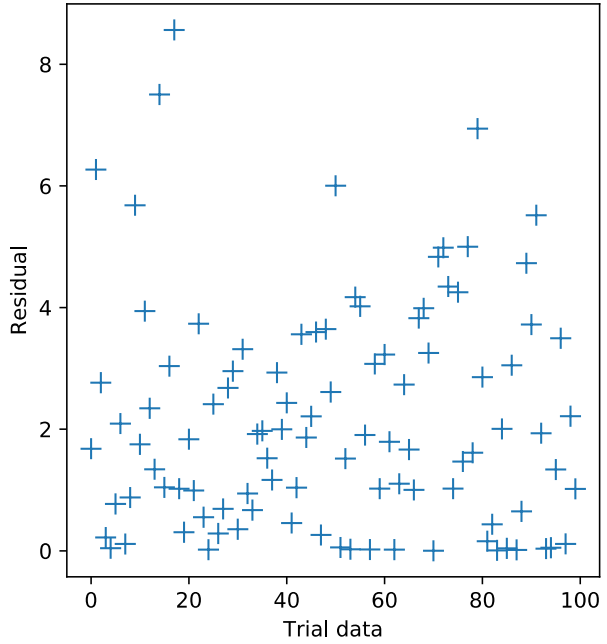
Signal analysis: Hidden layers size 3

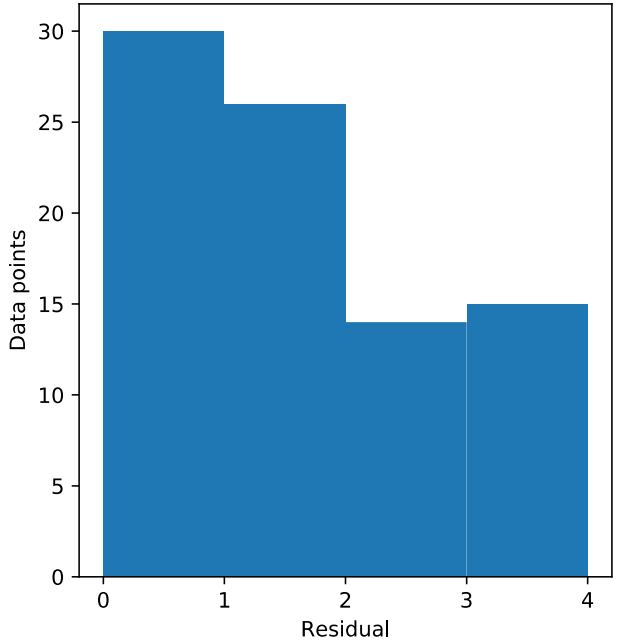
Test on the training set





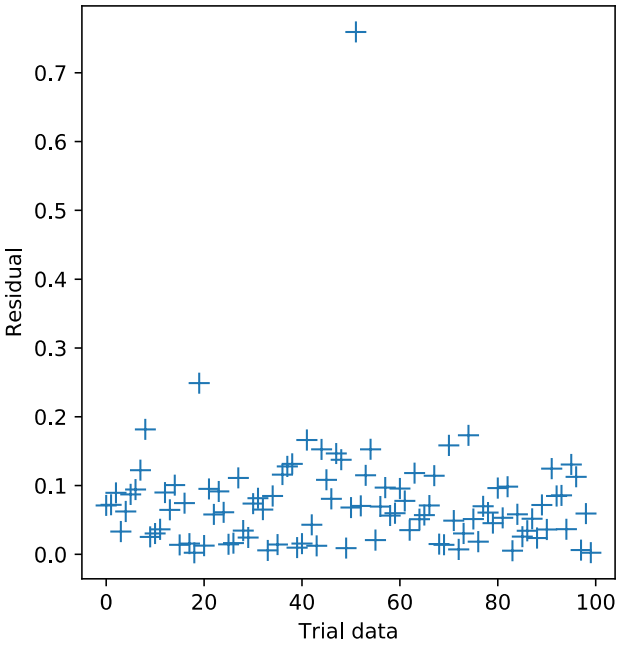
Test on new data

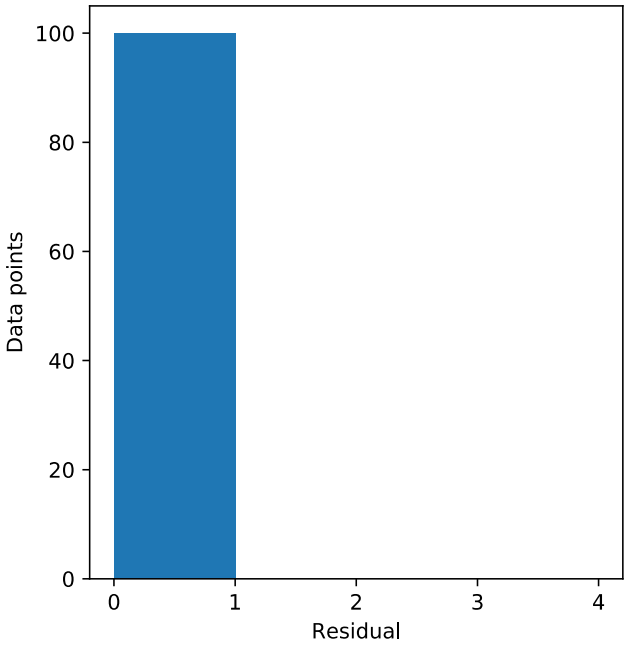




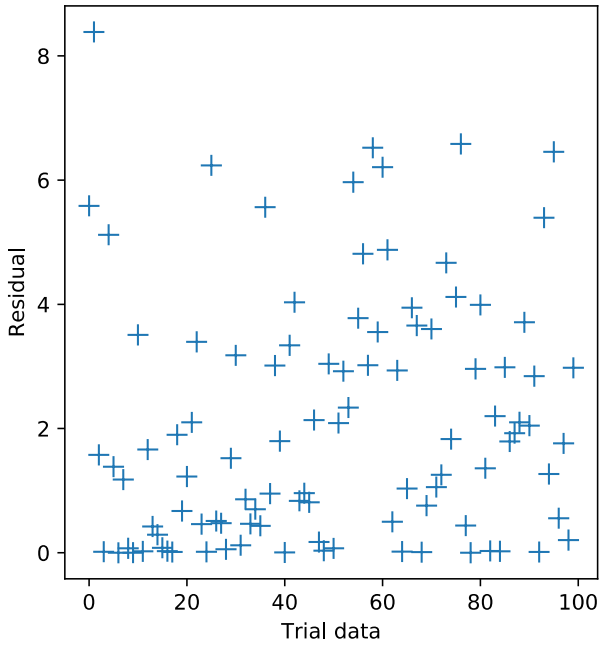
Signal analysis: Hidden layers size 4

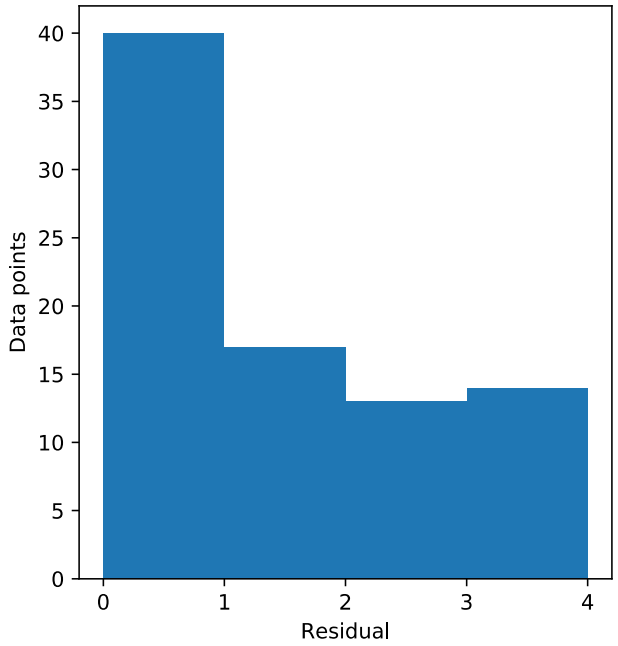
Test on the training set





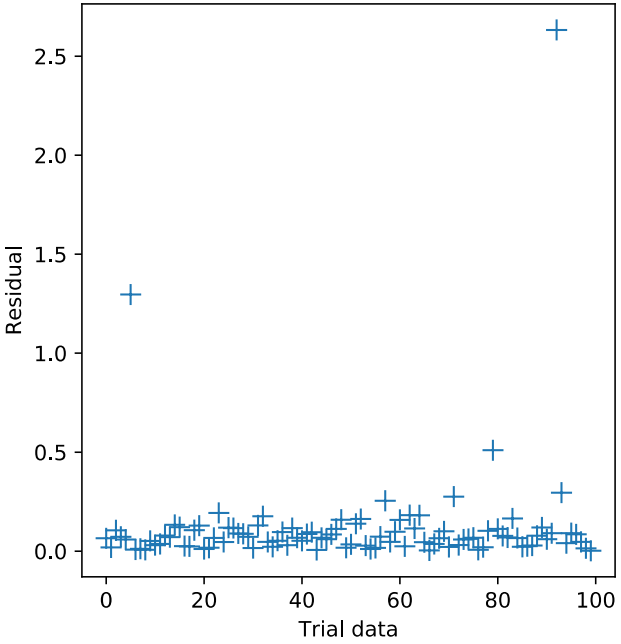
Test on new data

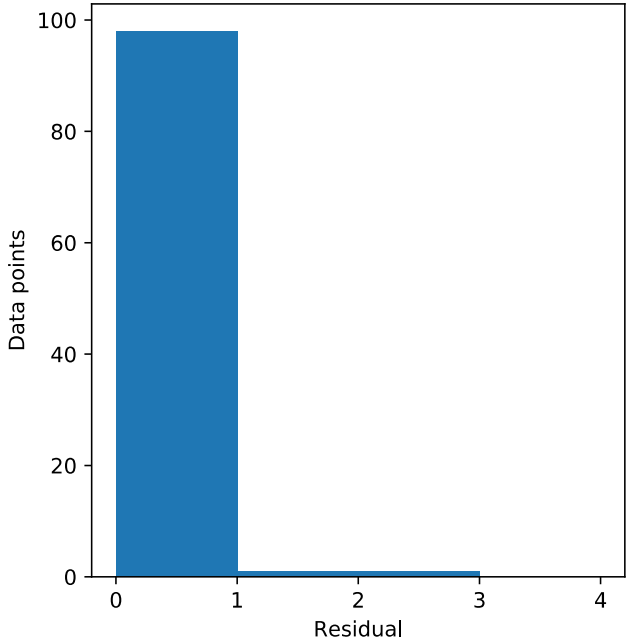




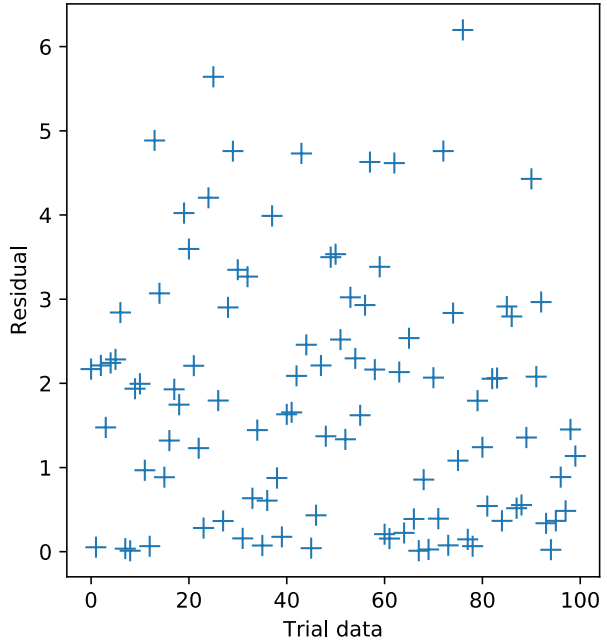
Signal analysis: Hidden layers size 8

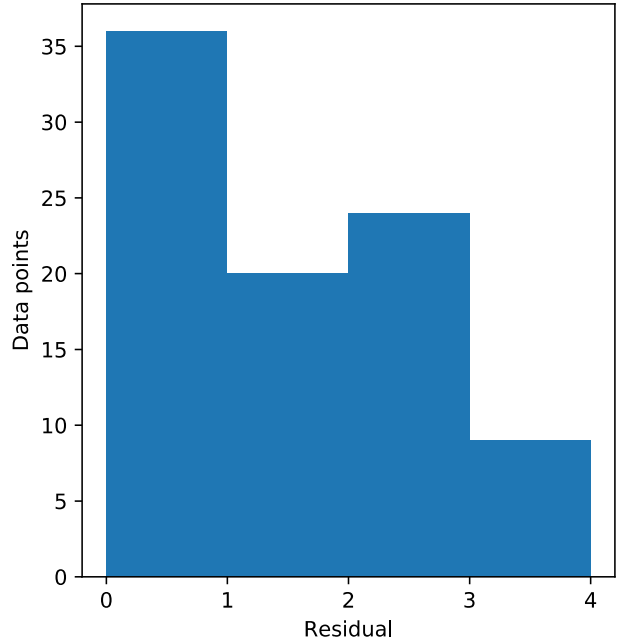
Test on the training set



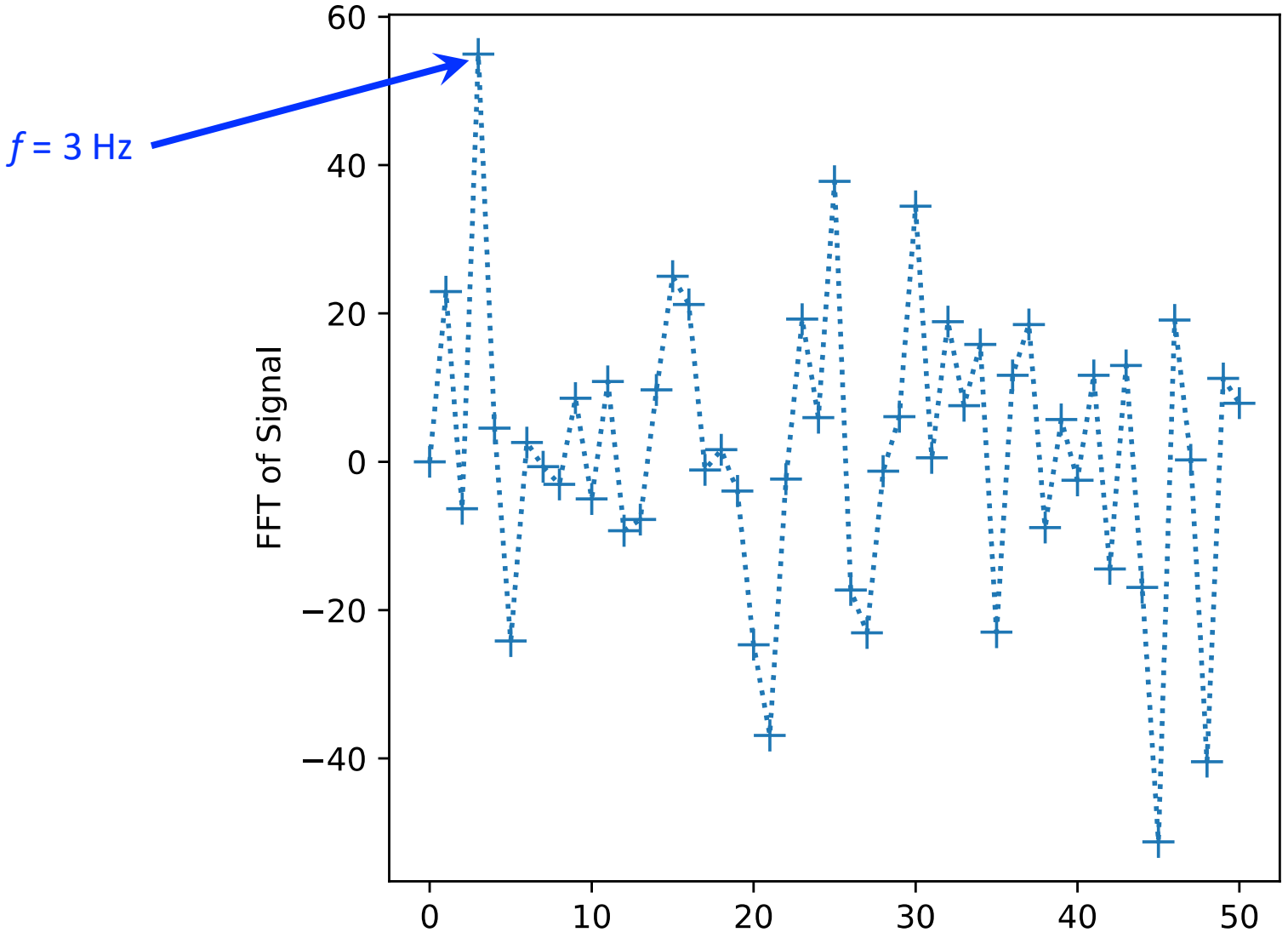


Test on new data





Can we do the same with an FFT?



After class tasks

- HW5 due tomorrow
- HW4 graded soon

- Readings:
  - *Computational Methods for Physics*, Joel Franklin, Chapter 14
  - *Make Your Own Neural Network*, Tariq Rashid
  - http://playground.tensorflow.org