020-dl-pca-ica

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1 Deep Learning, Linear Layers, and PCA/ICA

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This is a low-quality PDF conversion; to see the original notebook, please go to: github.com/tmbdev/dl-2018

The notebooks are directly executable.

In [1]:
```
%pylab inline
rc("image", cmap="gray", interpolation="nearest")
```

```
Populating the interactive namespace from numpy and matplotlib
```

In [2]:
```
# common imports
import os
import pickle
import matplotlib.pyplot as plt
import numpy as np
import scipy.ndimage as ndi
import sklearn
import torch
from graphviz import Source
from matplotlib import gridspec
from scipy.stats import kde
from sklearn import decomposition
from torch import nn, optim

import imgclass
import imgimg
```

In [3]:
```
# helper functions
def plot_density(data, nbins=100):
    x, y = data.T
    k = kde.gaussian_kde(data.T)
    xi, yi = np.mgrid[x.min():x.max():nbins*1j, y.min():y.max():nbins*1j]
    zi = k(np.vstack([xi.flatten(), yi.flatten()]))
```

```python
    pcolormesh(xi, yi, zi.reshape(xi.shape),
               shading='gouraud', cmap=plt.cm.BuGn_r)
    contour(xi, yi, zi.reshape(xi.shape))


def tshow(v, ax=None, **keys):
    if isinstance(v, torch.Tensor):
        v = v.cpu().detach().numpy()
    if v.ndim == 1:
        v = v.reshape(28, 28)
    if ax is not None:
        ax.imshow(v, **keys)
    else:
        imshow(v, **keys)


def showgrid(images, rows=4, cols=4, cmap=cm.gray, size=(6, 6)):
    if size is not None:
        figsize(*size)
    for i in range(rows*cols):
        subplot(rows, cols, i+1)
        xticks([])
        yticks([])
        tshow(images[i], cmap=cmap)


def showrow(*args):
    for i, im in enumerate(args):
        subplot(1, len(args), i+1)
        tshow(im)


def T(a):
    return torch.FloatTensor(a).cuda()


def N(a):
    return a.cpu().detach().numpy()


def center_rows(images):
    shape = images.shape
    images = images.reshape(len(images), -1)
    images = images - mean(images, axis=1)[:, newaxis]
    images /= norm(images, axis=1)[:, newaxis]
    images.reshape(*shape)
    return images
```

```
def flat_rows(images):
    return images.reshape(len(images), -1)
```

In [4]:
```
# download MNIST

!wget -nc -nd http://storage.googleapis.com/lpr-ocr/mnist.pyd.gz
data = pickle.load(os.popen("zcat mnist.pyd.gz"))
globals().update(data)
print images.shape, images.dtype, amax(images)

def load_images(images):
    #images = ndi.gaussian_filter(images, (0, 0.5, 0.5))
    images = center_rows(images)
    images = flat_rows(images)
    cuimages = torch.FloatTensor(images).cuda()
    return images, cuimages

images, cuimages = load_images(images)
cuclasses = torch.LongTensor(classes).cuda()
test_images, cutest_images = load_images(test_images)
cutest_classes = torch.LongTensor(test_classes).cuda()
print cuimages.shape
```

```
File 'mnist.pyd.gz' already there; not retrieving.

(60000, 28, 28) float32 1.0
torch.Size([60000, 784])
```

In [5]:
```
# display helpers


def display_components(a, l, fs=None, rows=1, row=0, yscale="log", ylim=None):
    fig = plt.figure(figsize=fs)
    outer = gridspec.GridSpec(rows, 2, wspace=0.2, hspace=0.2)
    inner = gridspec.GridSpecFromSubplotSpec(4, 4,
                                             subplot_spec=outer[2*row], wspace=0.1, hspa
    for j in range(16):
        ax = plt.Subplot(fig, inner[j])
        image = a[j]
        if isinstance(a, (torch.Tensor, torch.cuda.FloatTensor)):
            a = N(a)
        if image.ndim == 1:
            image = image.reshape(len(image)//28, 28)
        ax.imshow(image, cmap=cm.RdBu)
        ax.set_xticks([])
        ax.set_yticks([])
```

```
            fig.add_subplot(ax)

        if l is not None:
            ax = plt.Subplot(fig, outer[2*row+1])
            ax.plot(l)
            ax.set_yscale(yscale)
            if ylim is not None:
                ax.set_ylim(ylim)
            fig.add_subplot(ax)

        if False:
            ax = plt.Subplot(fig, outer[2])
            ax.imshow(dot(a, a.T))
            fig.add_subplot(ax)


    def plot_pca_variance(data, k, **kw):
        pca = decomposition.PCA(k)
        pca.fit(data.reshape(len(data), -1))
        plot(pca.explained_variance_, **kw)
```

2 Introduction

In this section, we are going to look at the relationship between linear methods, linear subspaces, and deep learning.

This is complementary to recent methods of analyzing neural networks like… - deep dreaming - layer reconstruction - "manifold"-based arguments

Why? - the linear theory is the basis for the non-linear theory ("manifolds") - the linear theory is well-developed (independence, optimal coding, etc.) - we can find optimal solutions to various problems (e.g., linear reconstructions) - you should know the linear theory - these are practical, deterministic tools for analyzing neural network layers

3 Simple PCA

3.1 PCA

Principal Component Analysis solves the following problem:

Find a matrix $W \in \mathbb{R}^{k \times n}$ that is orthonormal $ W W^T = 1 $ that minimize reconstruction error

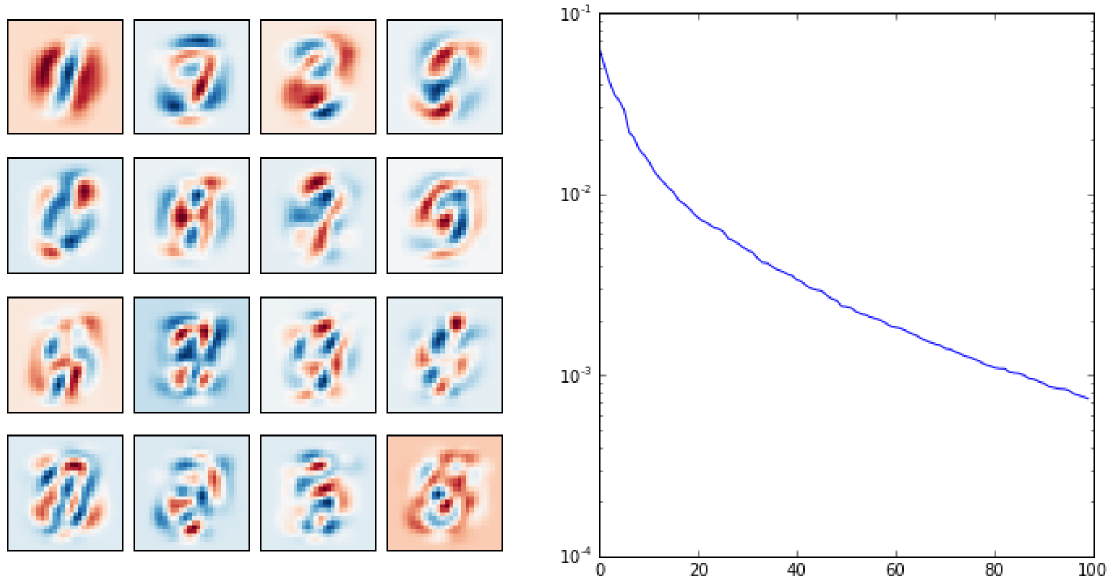
$$\sum ||W^T W x_i - x_i||^2$$

I.e., represent some collection of vectors in an optimal way in a subspace.

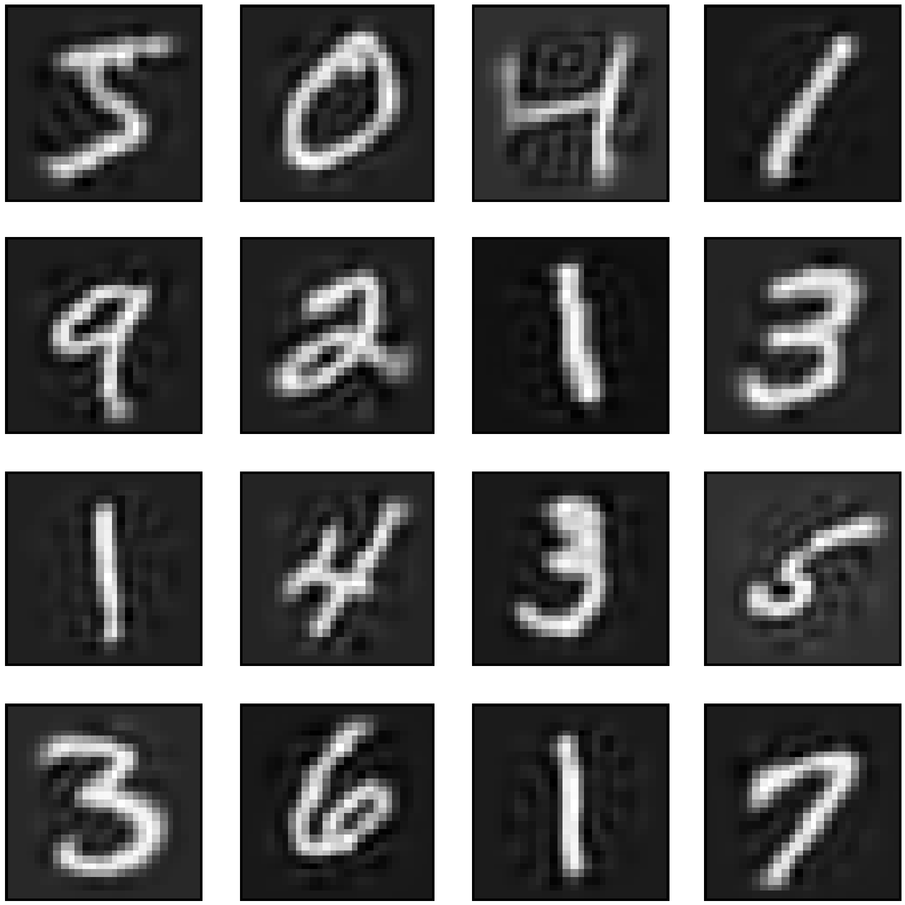
```
In [6]: # compute a PCA and display the components

        def show_pca(data, n_pca=100, **kw):
            pca = decomposition.PCA(n_pca)
            pca.fit(data.reshape(len(data), -1))
```

```
        display_components(pca.components_, pca.explained_variance_, **kw)
        return pca
```

In [7]:
```
# PCA - learn to recognize these shapes
pca = show_pca(images, 100, fs=(12,6))
```



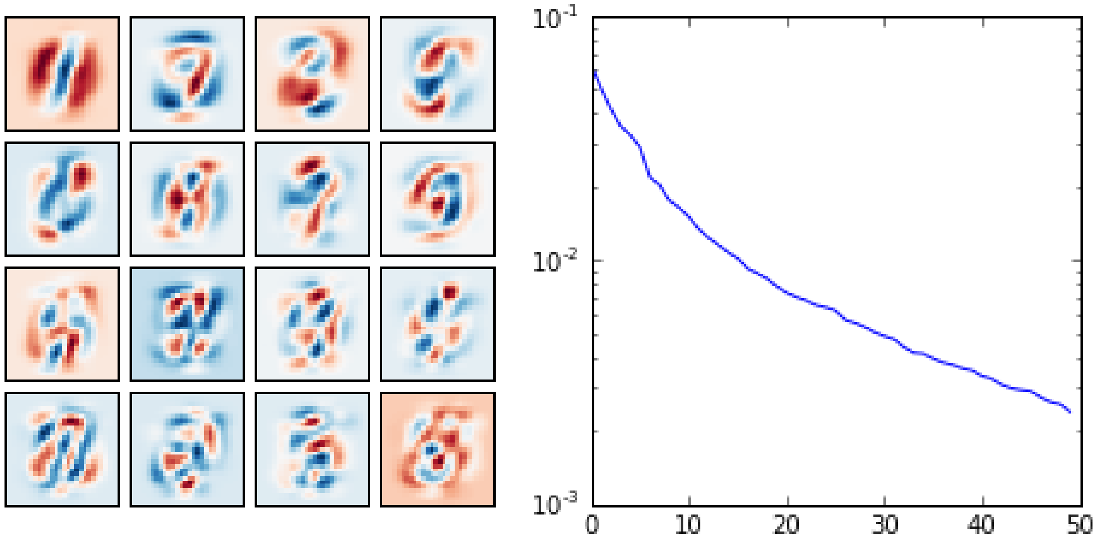
In [8]:
```
# project onto the transform's subspace then project back

def tproject(f, inputs):
    return f.inverse_transform(f.transform(inputs))

showgrid(tproject(pca, images))
```

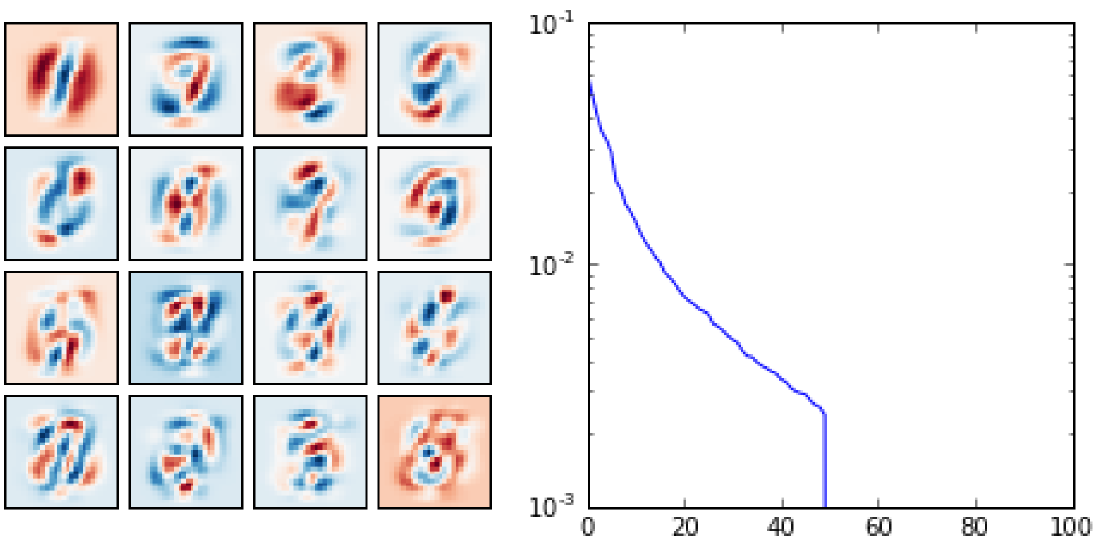


In [9]: # after a first PCA, the components are "just gone" in a second PCA

```
figsize(8,8)
pca = show_pca(images, 50, rows=2, row=0, ylim=(1e-3, 1e-1))
pca2 = show_pca(tproject(pca, images), 100, rows=2, row=1, ylim=(1e-3, 1e-1))
```

summary





PCA finds an optimal (L2 sense) linear subspace for representing the input.

PCA consists of a rotation, a projection, and a measure of variances in each direction. When data exists in a linear subspace, the variances drop to zero.

4 ICA Subspaces

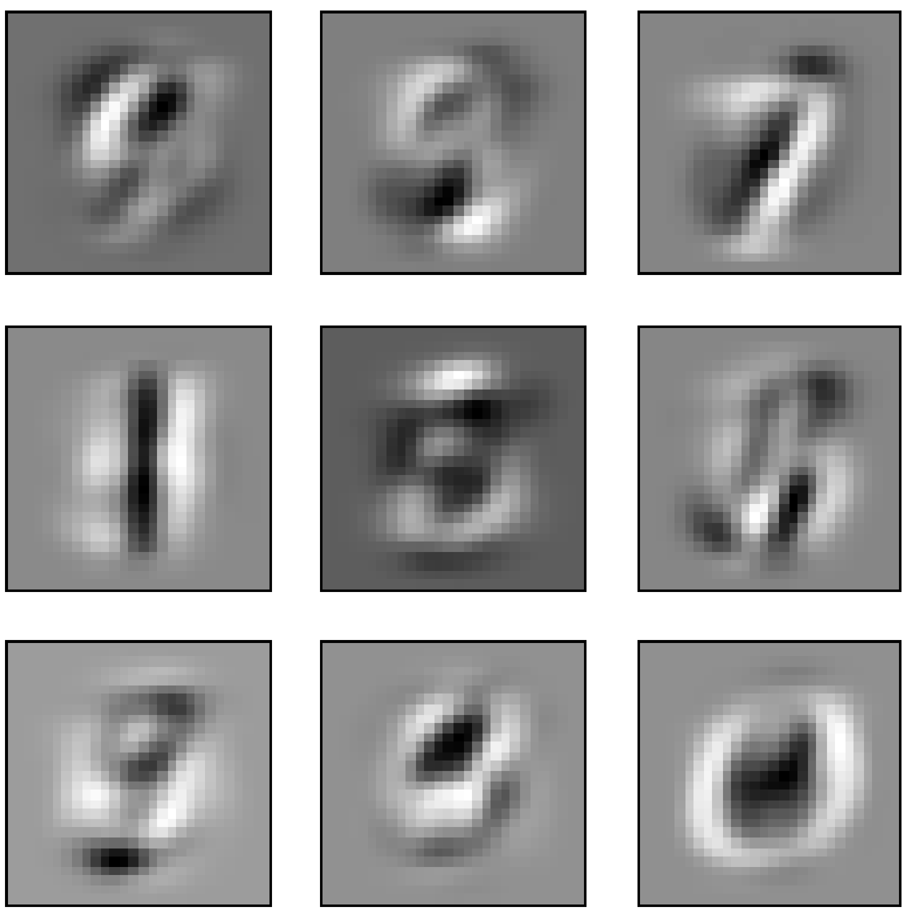
4.1 Independent Component Analysis

Find a matrix $W \in \mathbb{R}^{k \times n}$ that is orthonormal $ W W^T = 1 $ that minimize reconstruction error

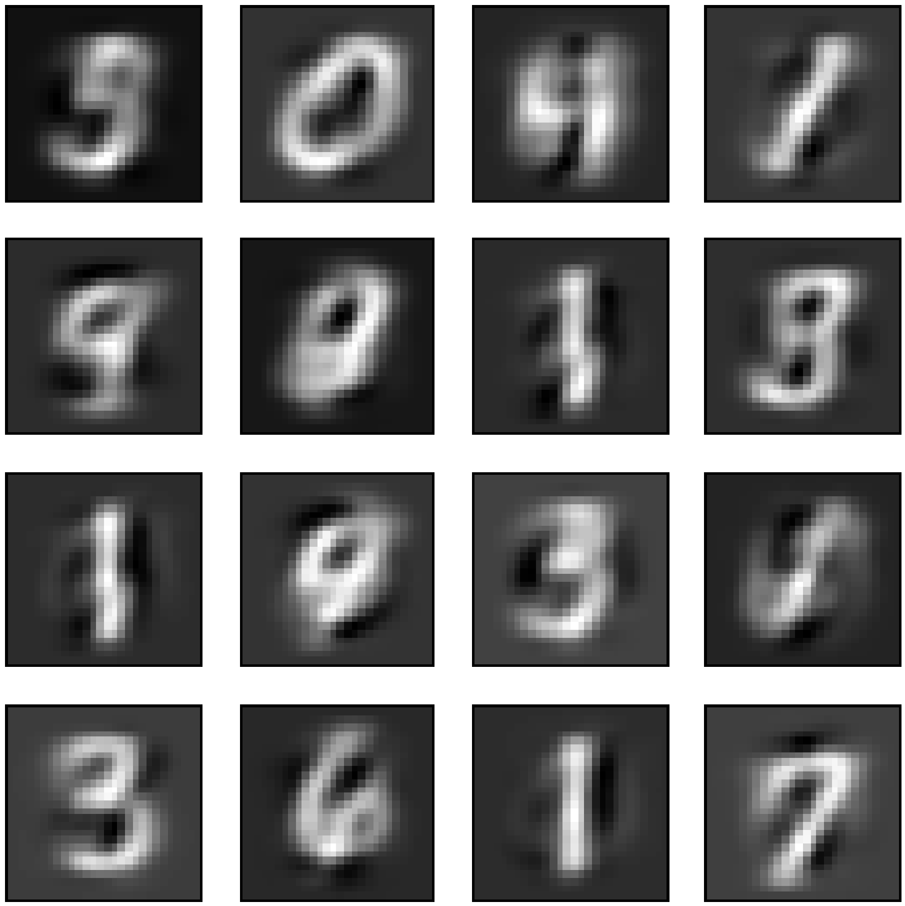
- the components of $W \cdot x$ have minimal mutual information
- the components of $W \cdot x$ are maximally non-Gaussian
- that minimizes $\sum ||W \cdot x||_1$

```
In [10]: k = 9
         ica0 = decomposition.FastICA(k)
         ica0.fit(images.reshape(len(images), -1))
         ica0_basis = ica0.inverse_transform(diag(ones(k))).reshape(k, 28, 28)
         showgrid(ica0_basis, 3, 3)
```

```
/opt/conda/lib/python2.7/site-packages/sklearn/decomposition/fastica_.py:118: UserWarning: FastI
  warnings.warn('FastICA did not converge. Consider increasing '
```

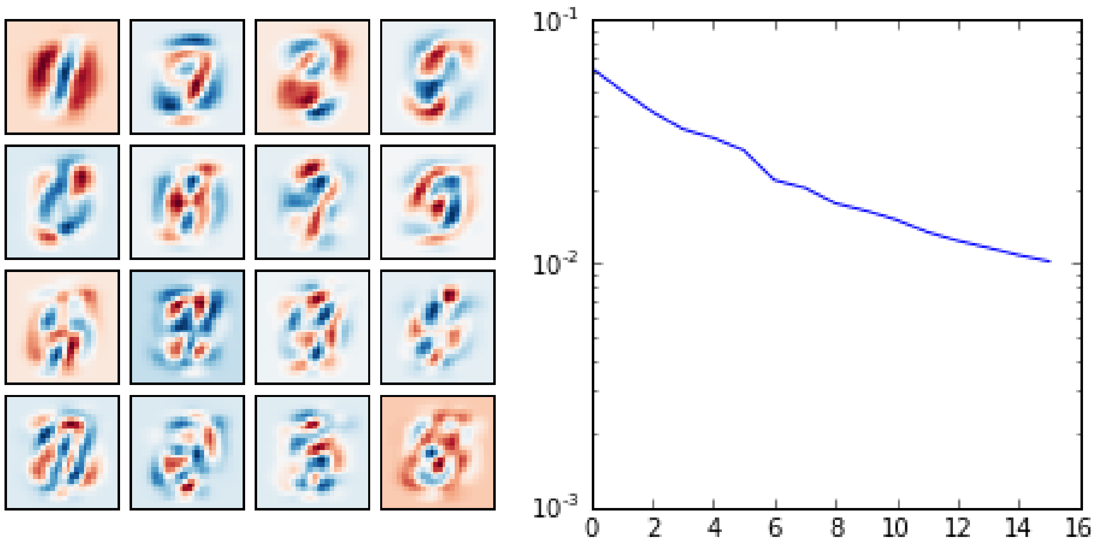


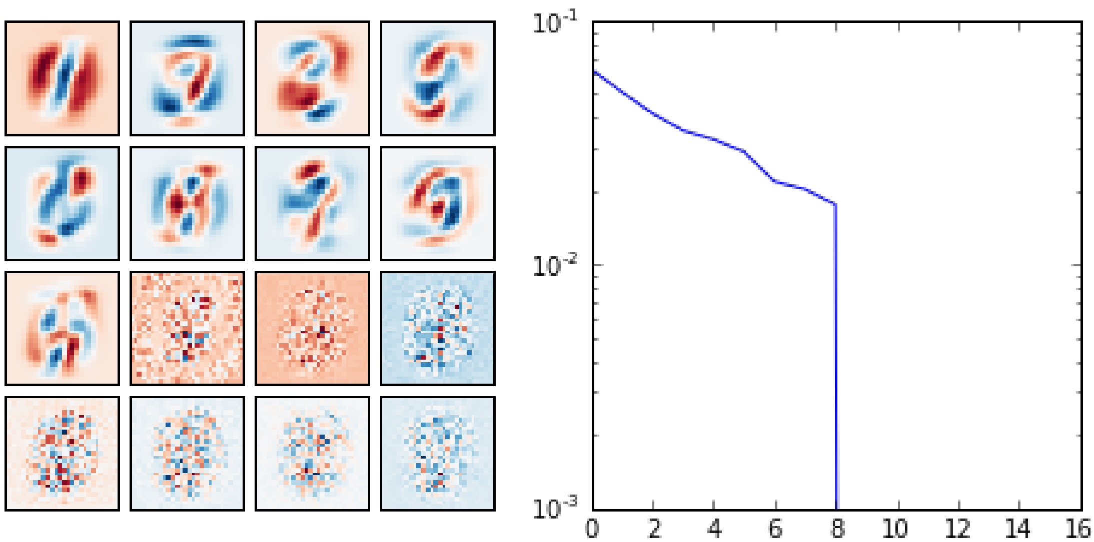
```
In [11]: ica0_recon = tproject(ica0, images)
         showgrid(ica0_recon)
```



```
In [12]: figsize(8,8)
         show_pca(images, 16, rows=2, row=0, ylim=(1e-3, 1e-1))
         show_pca(ica0_recon, 16, rows=2, row=1, ylim=(1e-3, 1e-1))

Out[12]: PCA(copy=True, iterated_power='auto', n_components=16, random_state=None,
           svd_solver='auto', tol=0.0, whiten=False)
```

summary

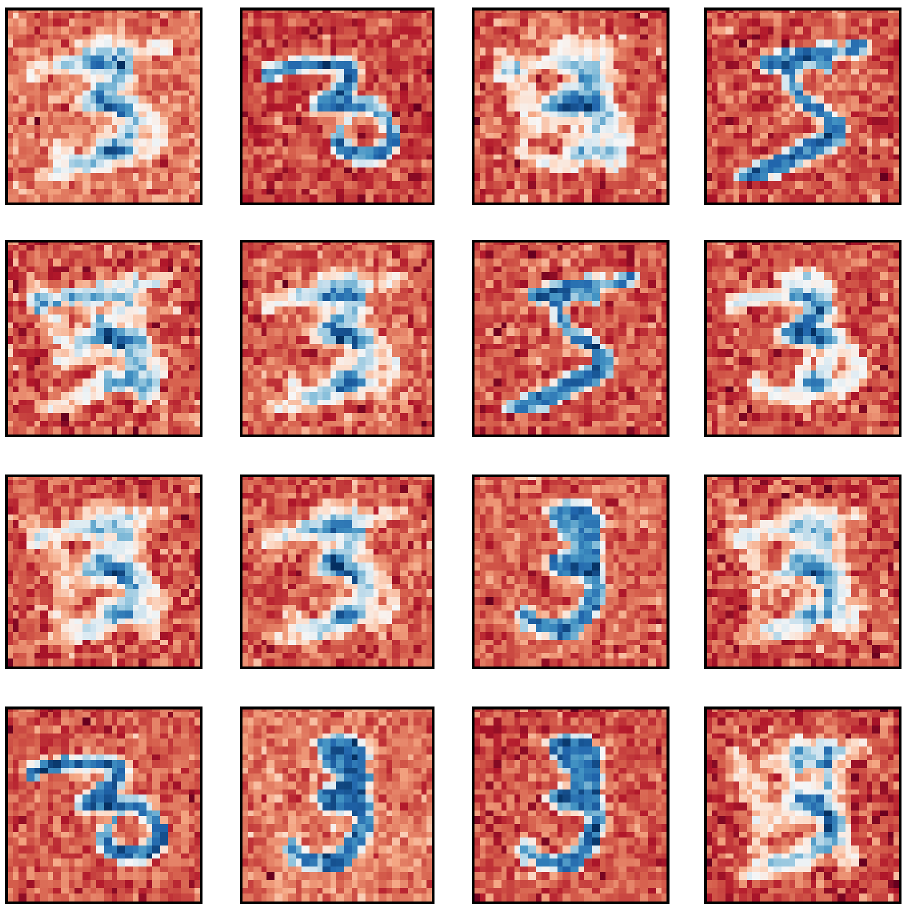




ICA finds another low-dimensional subspace, with maximum non-Gaussian components. The ICA space is still a low-dimensional linear subspace, which shows up in PCA analysis.

5 The Cocktail Party Problem

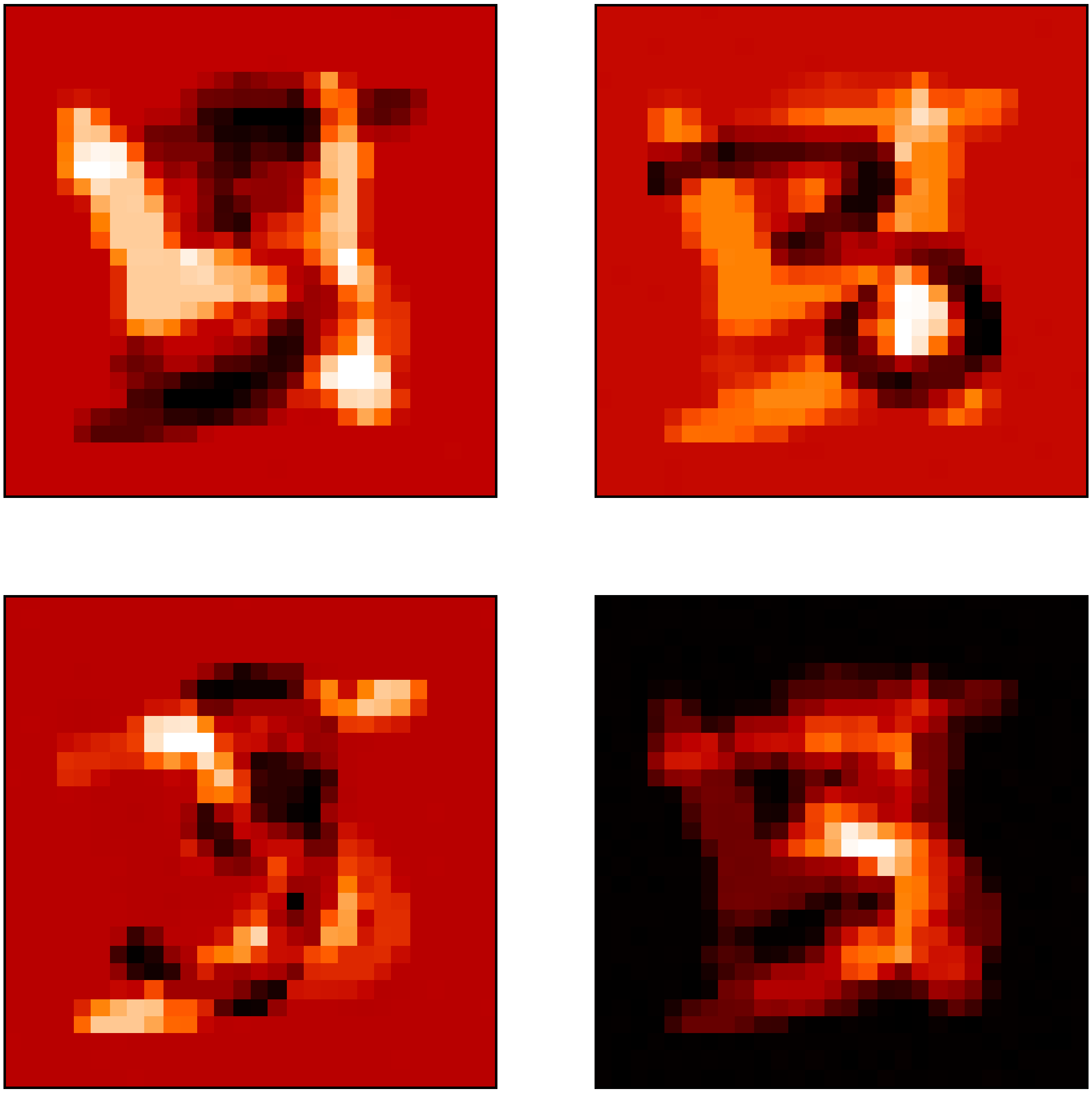
In [13]:
```
k = 4
mps = (rand(50000, k) < 0.5) + 0.01
mps = mps / mps.sum(1)[:, newaxis]
mixture = dot(mps, images[:10*k:10])
mixture = mixture + 0.01 * randn(*mixture.shape)
mixture = center_rows(mixture)
showgrid(mixture, cmap=cm.RdBu)
```



PCA finds the optimal representation in terms of reconstruction error.

In [14]:
```
pca = decomposition.PCA(k)
pca.fit(mixture)
for i in range(4):
    if median(pca.components_[i])>0:
```

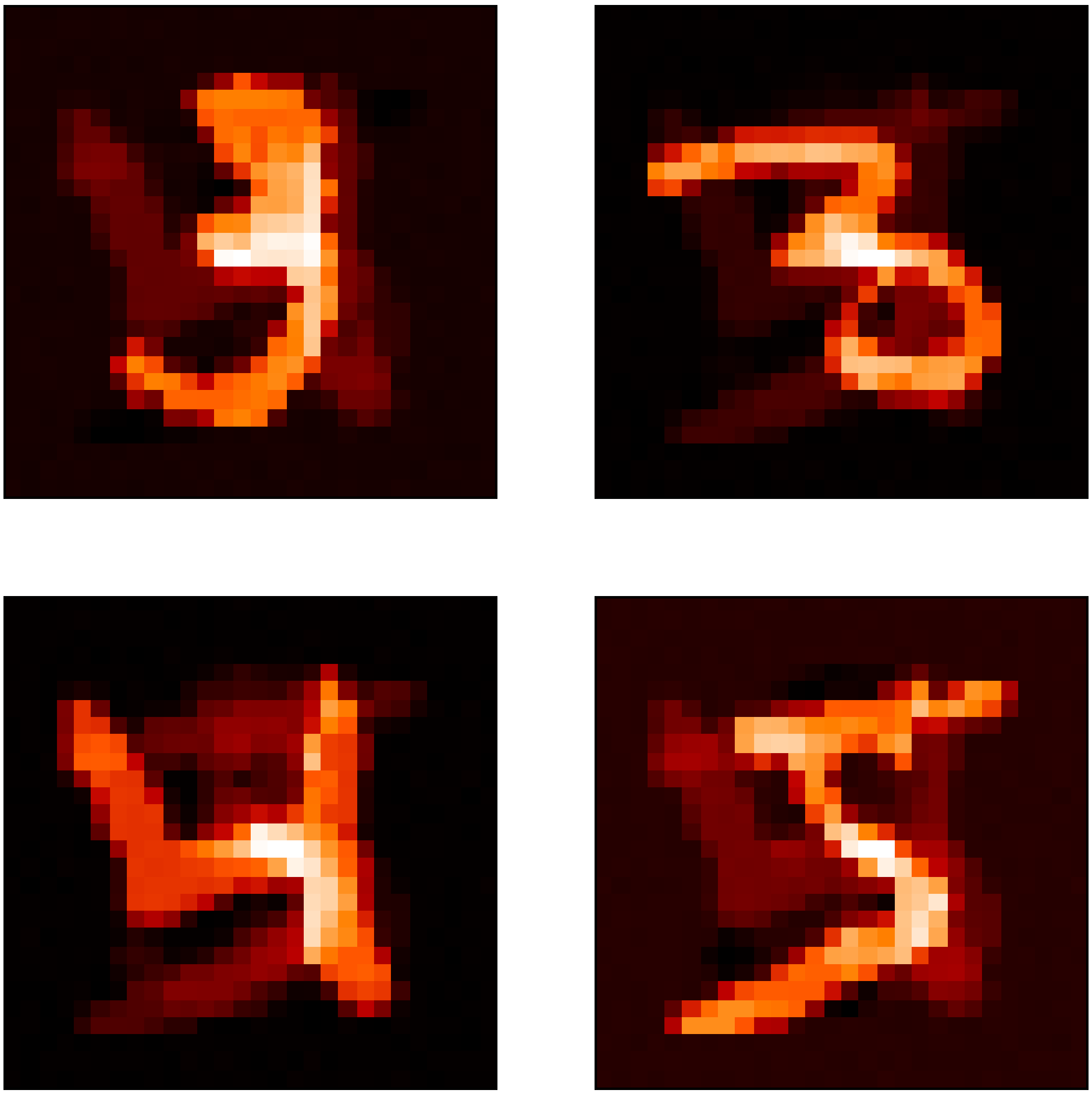
```
        pca.components_[i] = - pca.components_[i]
showgrid(pca.components_, cmap=cm.gist_heat, size=(8,8), rows=2, cols=2)
```



ICA recovers the independent components instead.

```
In [15]: ica = decomposition.FastICA(k)
         ica.fit(mixture)
         for i in range(4):
             if median(ica.components_[i])>0:
                 ica.components_[i] = - ica.components_[i]
         showgrid(ica.components_, cmap=cm.gist_heat, size=(8,8), rows=2, cols=2)
```

summary



ICA can separate “mixed sources”.

Equivalently, here, each image component has a non-Gaussian (specifically, binomial) distribution.

This can be an important factor in explaining low level feature extraction in images.

6 Reconstruction ICA

6.1 Reconstruction ICA (RICA) Definition

ICA is an odd data transformation because it doesn't make reference to actually preserving any of the data. We can come up with an alternative definition based on *reconstruction loss*:

$\hat{W} = \arg\min_w \lambda ||WX||_1 + ||W^T W x - x||_2^2$

We may still constraint $W^T W = \mathbb{1}$.

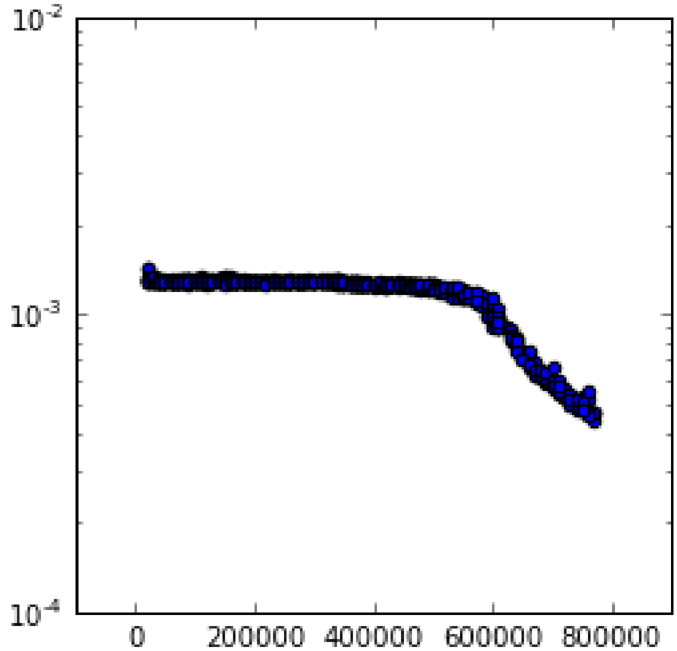
- For $\lambda \to \infty$ and whitened data, this is equivalent to ICA.
- For $\lambda = 0$, this is simply PCA or a linear autoencoder.

This can be implemented directly as a neural network.

In [16]:
```
def orthocost(a):
    return ((torch.mm(a, a.transpose(1, 0))-torch.eye(a.size(0)).cuda())**2).sum()

def l1cost(y):
    return (y.abs().sum(1)-1).abs().sum()
```

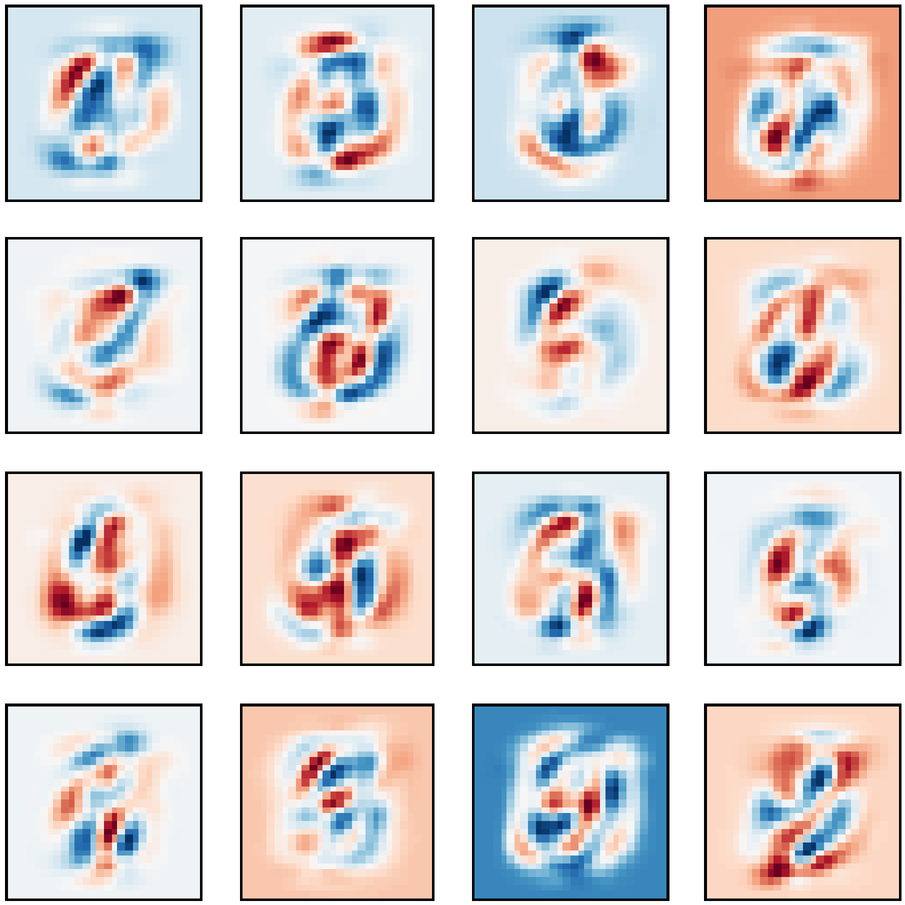
In [17]:
```
class RICA(nn.Module):
    def __init__(self):
        nn.Module.__init__(self)
        self.weight = nn.Parameter(1e-4 * torch.rand(50, 28*28))
    def forward(self, x):
        y = self.weight.mm(x.transpose(1,0))
        z = self.weight.transpose(1,0).mm(y).transpose(1, 0)
        cost = 0
        cost = cost + 1e-5 * l1cost(y)
        #cost = cost + 1e-5 * orthocost(self.weight)
        return z, cost

def make_model(): return RICA().cuda()
```

In [18]:
```
cuimages = torch.FloatTensor(images).cuda()
amlp = imgimg.AutoMLP(make_model, cuimages, cuimages, initial_bs=100, maxtrain=1000000)
rica = amlp.train()
```




```
<matplotlib.figure.Figure at 0x7f801432a5d0>
```

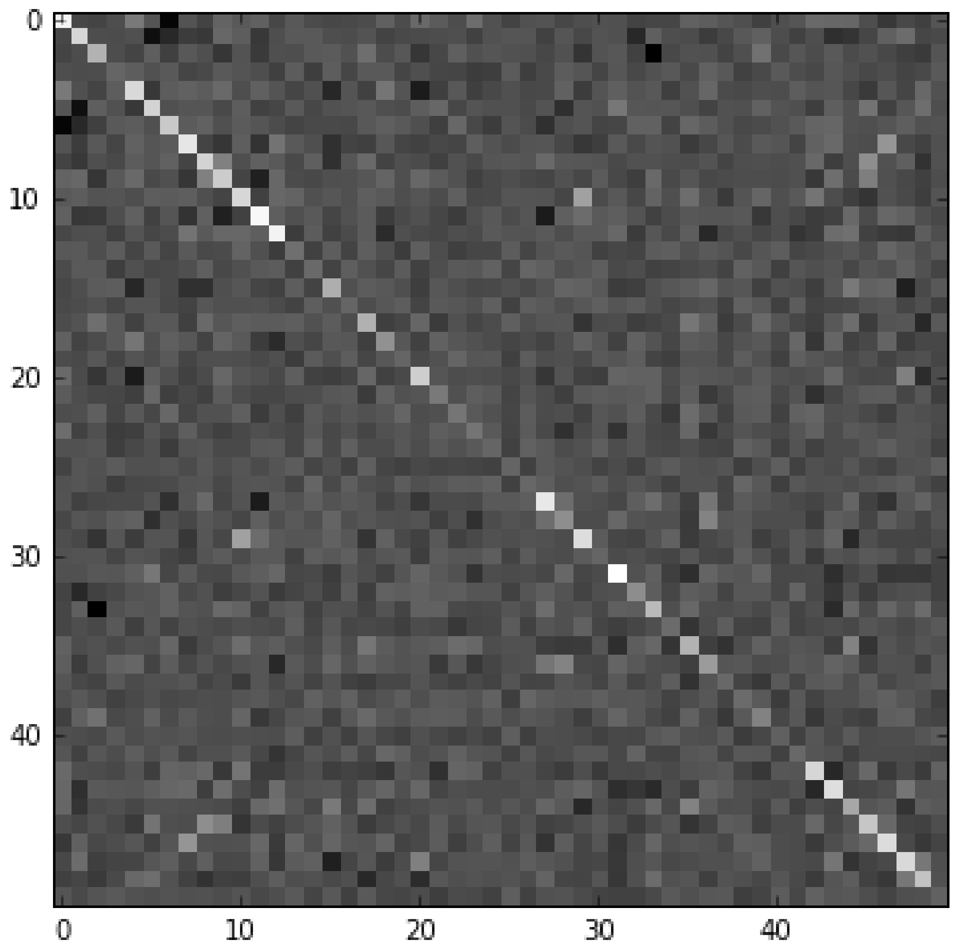
```
In [19]: showgrid(rica.weight, cmap=cm.RdBu)
```



```
In [20]: imshow(N(rica.weight.mm(rica.weight.transpose(1, 0))))
```

```
Out[20]: <matplotlib.image.AxesImage at 0x7f8010d91f10>
```

summary



ICA can be formulated as a “neural learning algorithm” similar to PCA as “RICA”

The loss function in RICA is a combination of reconstruction loss (as in PCA) and an L1 loss on the activation of the encoding.

RICA can smoothly interpolate between optimal reconstruction (PCA) and independent components (ICA).

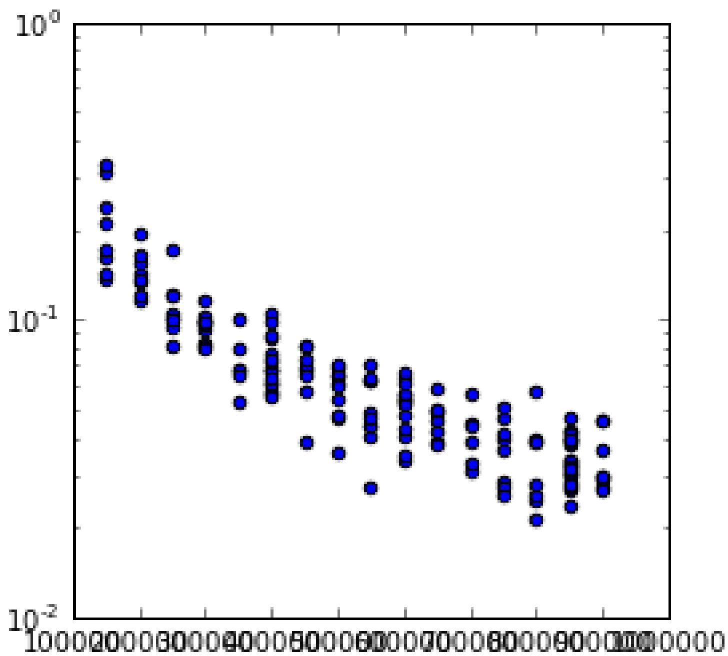
L1 losses imposed on hidden layers generate sparsity and favor non-Gaussian component selection.

7 Analyzing Hidden Layers

7.1 Training a Fully Connected Model

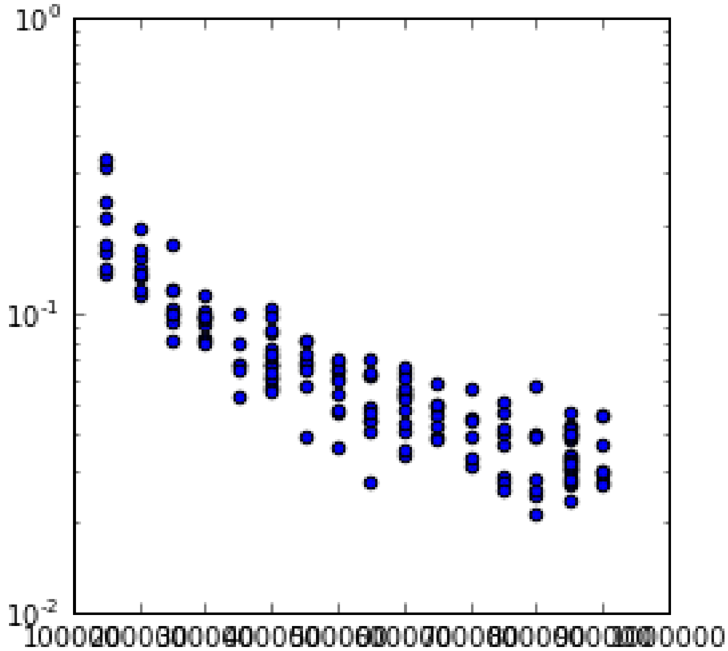
In [21]:
```
def make_model():
    return nn.Sequential(nn.Linear(28*28, 100),
                         nn.Sigmoid(),
                         nn.Linear(100, 10))
```

In [22]:
```
amlp = imgclass.AutoMLP(make_model, cuimages, cuclasses, cutest_images, cutest_classes,
                        initial_bs=20, maxtrain=1000000)
nn100 = amlp.train()
nn100.cuda()
```



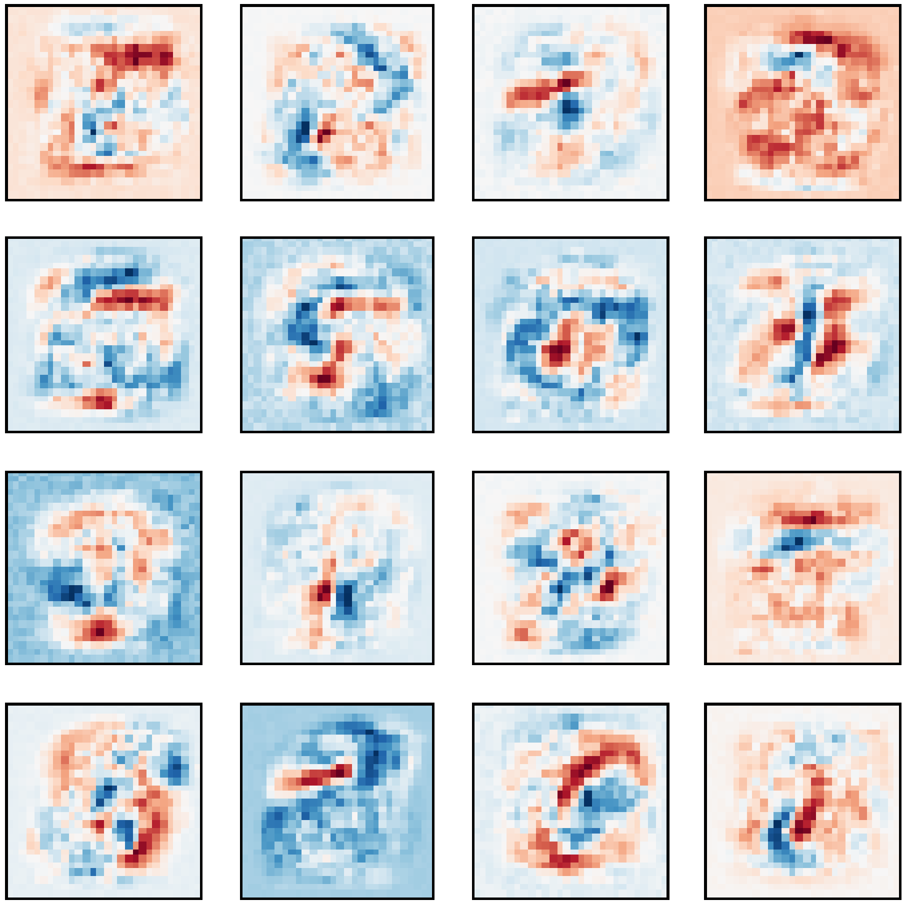

```
#best 0.021 @ 800000 of 900000
```

Out[22]:
```
Sequential(
  (0): Linear(in_features=784, out_features=100, bias=True)
  (1): Sigmoid()
  (2): Linear(in_features=100, out_features=10, bias=True)
)
```



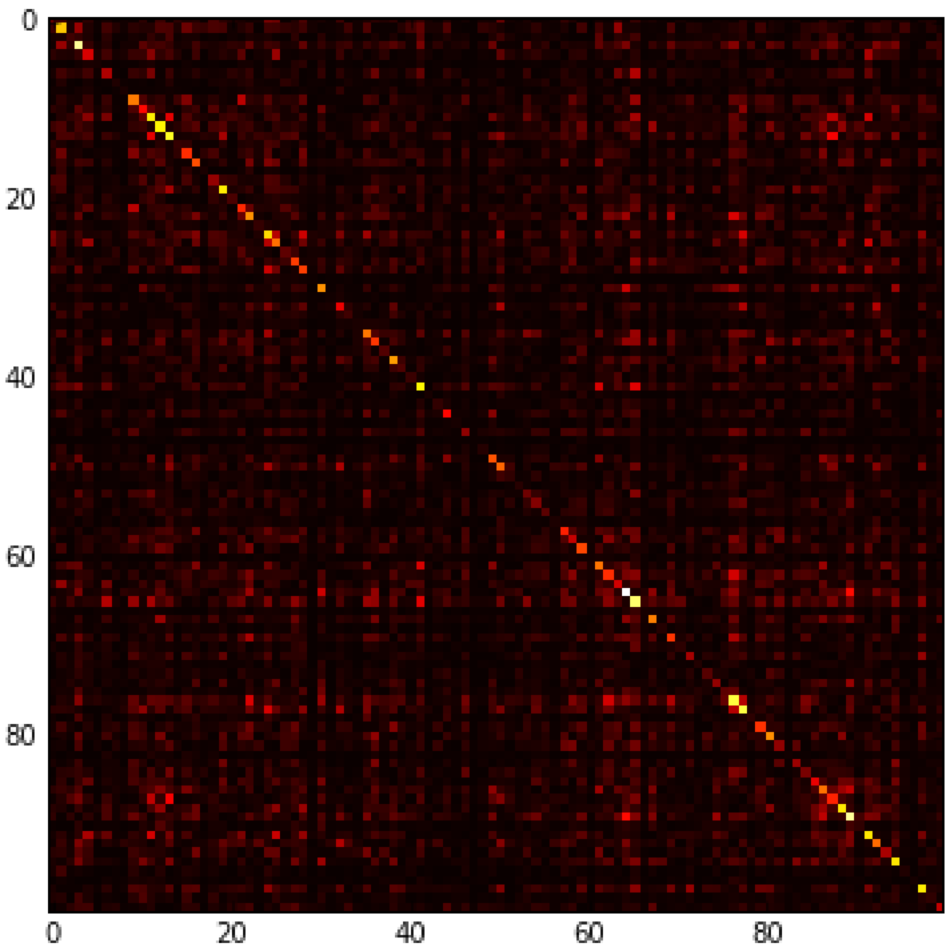

```
In [23]: nn100 = amlp.best_model
```

```
In [24]: W = N(nn100[0].weight)
         showgrid(W, cmap=cm.RdBu)
```



```
In [25]: imshow(abs(dot(W, W.T)), cmap=cm.hot)

Out[25]: <matplotlib.image.AxesImage at 0x7f801e077d90>
```

summary



Input units tend towards being imperfectly orthonormal (up to a scale factor). To the degree that input layers approximate a PCA, the vectors are mixed.

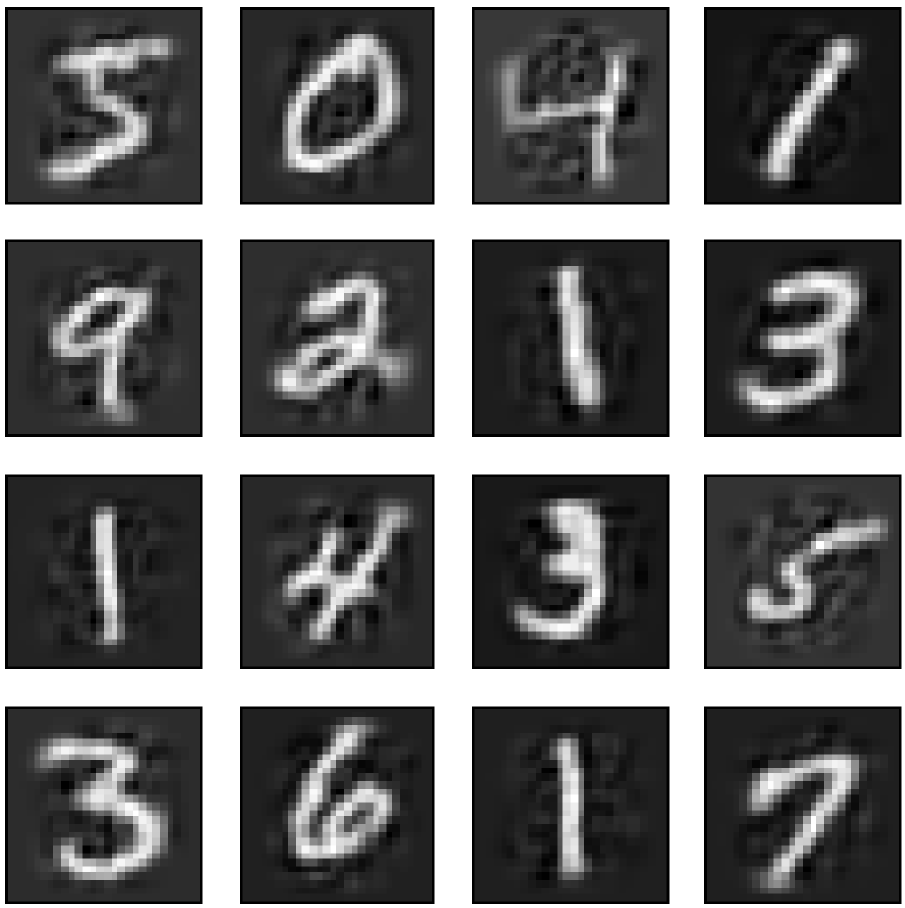
7.2 Output of the First Linear Layer

```
In [26]: nn100.cuda()
```

```
Out[26]: Sequential(
           (0): Linear(in_features=784, out_features=100, bias=True)
```

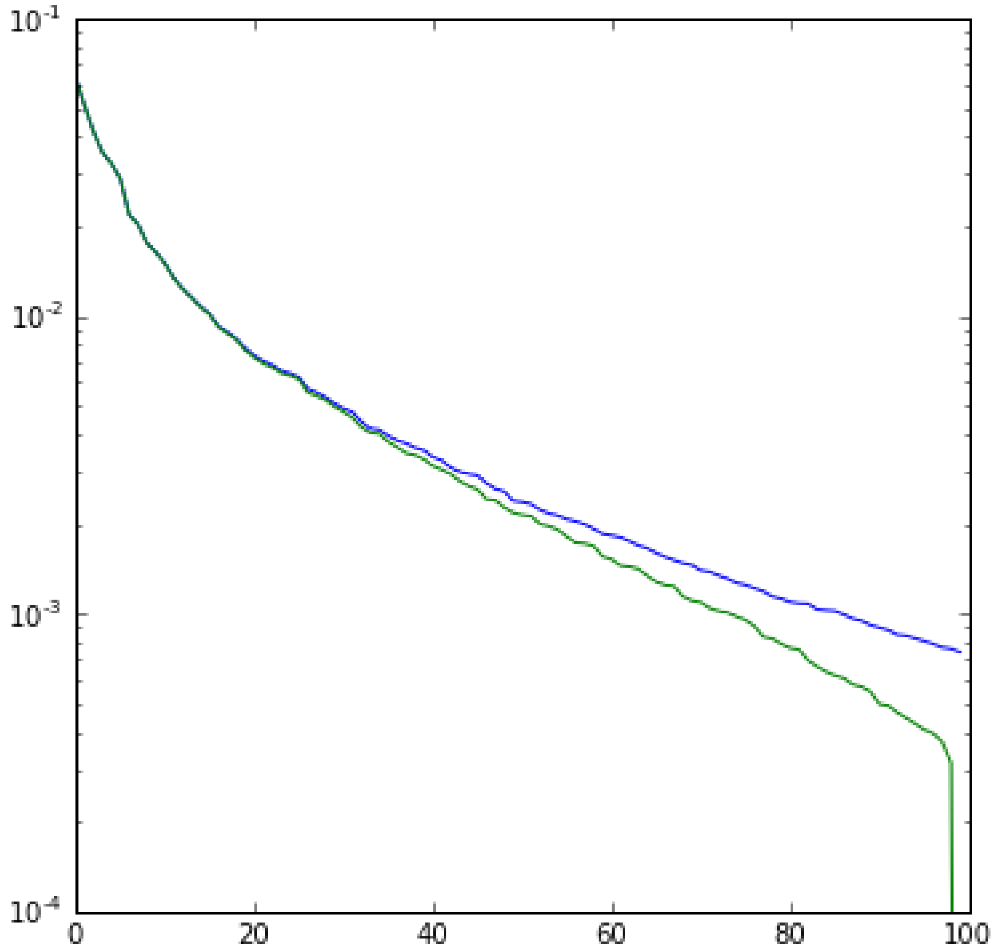
```
  (1): Sigmoid()
  (2): Linear(in_features=100, out_features=10, bias=True)
)
```

In [27]:
```
# run data through the first linear layer
nn100first_layer = N(nn100[0](cuimages))

# reconstruct the original images by mapping the linear output back to the input images
nn100recon = dot(nn100first_layer, dot(pinv(nn100first_layer), images))

showgrid(nn100recon)
```



In [28]:
```
yscale("log")
ylim((1e-4, 1e-1))
plot_pca_variance(images, 100)
plot_pca_variance(nn100recon, 100)
```

summary



We can use the pseudo-inverse to reconstruct inputs from hidden layer outputs.

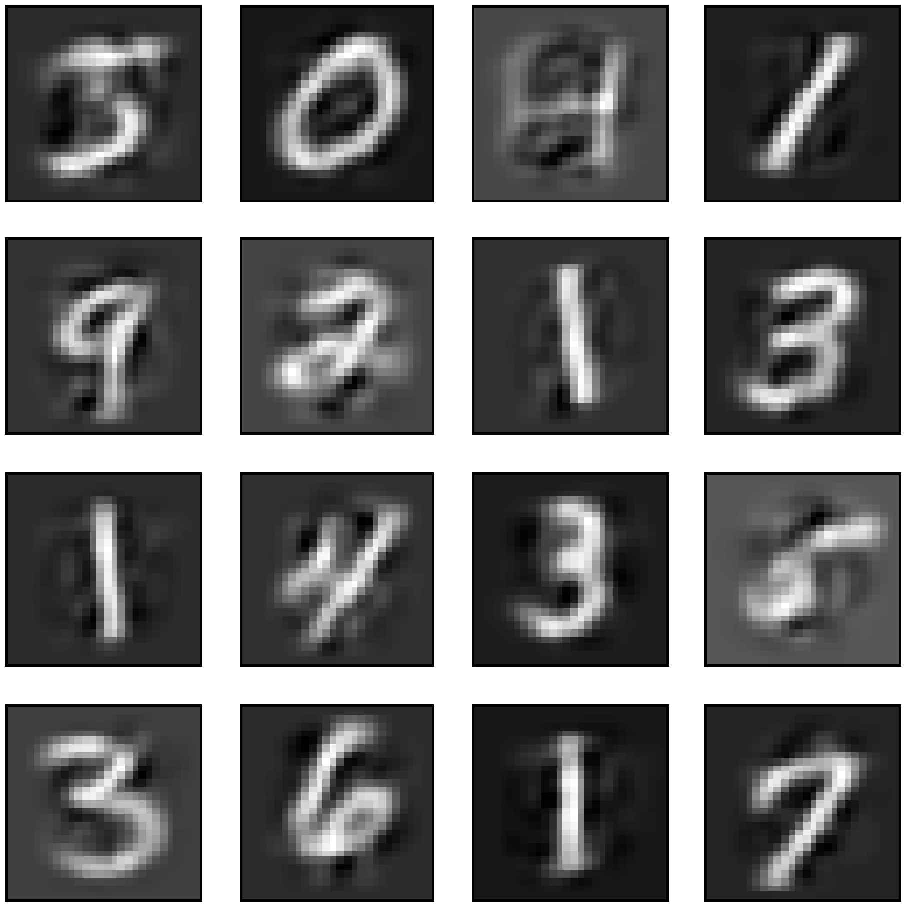
The generalization of this approach is to try to invert hidden layers by training another neural network.

Inputs are easily reconstructible from the output of the first linear layer.

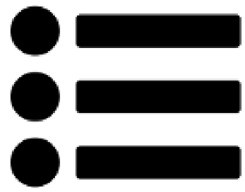
Most of the variance is accounted for in the output of the linear layer.

7.3 Output of the First Nonlinear Layer

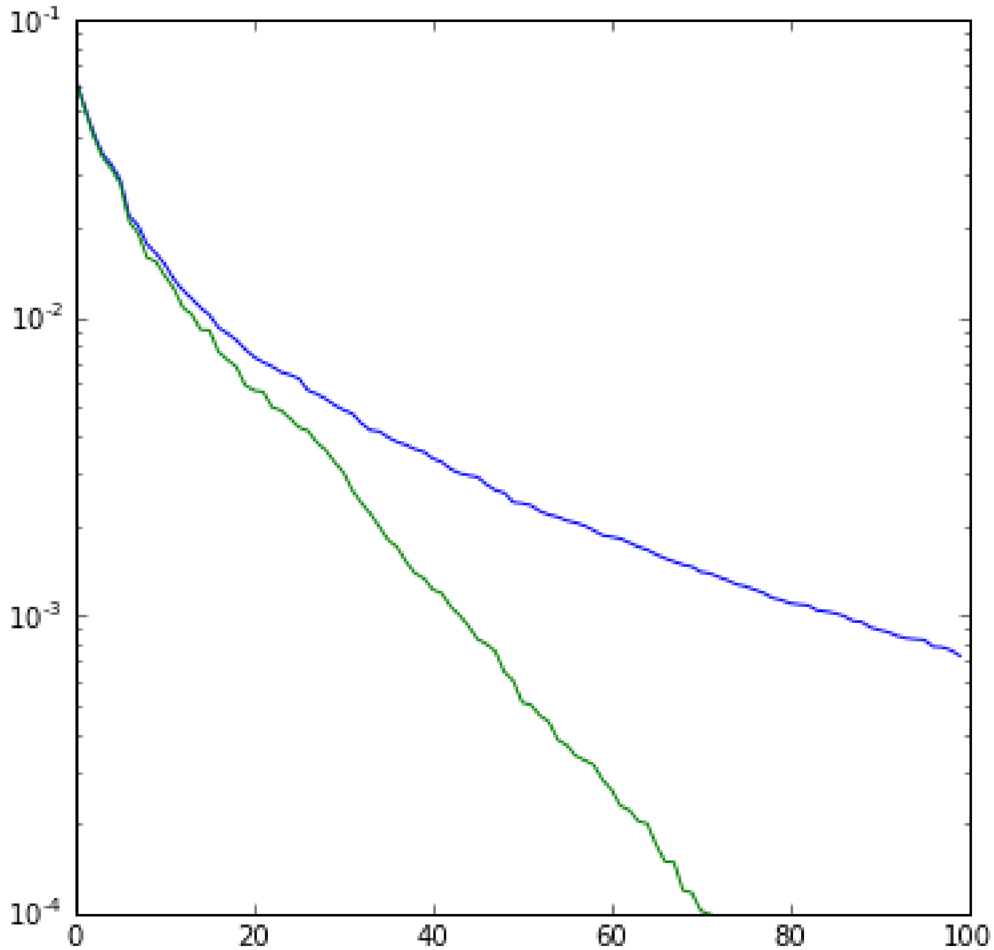
```
In [29]: nn100lin = N(nn100[0](cuimages))
         nn100nonlin = N(nn.Sequential(nn100[:2])(cuimages))
         nn100recon2 = dot(nn100nonlin, dot(pinv(nn100nonlin), images))
         showgrid(nn100recon2)
```



```
In [30]: yscale("log"); ylim((1e-4, 1e-1))
         plot_pca_variance(images, 100)
         plot_pca_variance(nn100recon2, 100)
```



summary



Information loss happens in the non-linear layer.

7.4 Non-Gaussianity via Kurtosis

Can we decide whether input layers are performing PCA or ICA?

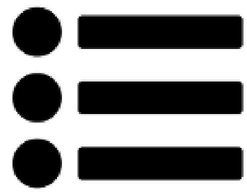
```
In [31]: pca = decomposition.PCA(100)
         pca.fit(images.reshape(len(images), -1))
         ica = decomposition.FastICA(100)
```

```
        ica.fit(images.reshape(len(images), -1))
        ica_basis = ica.inverse_transform(diag(ones(100))).reshape(100, 28, 28)
```

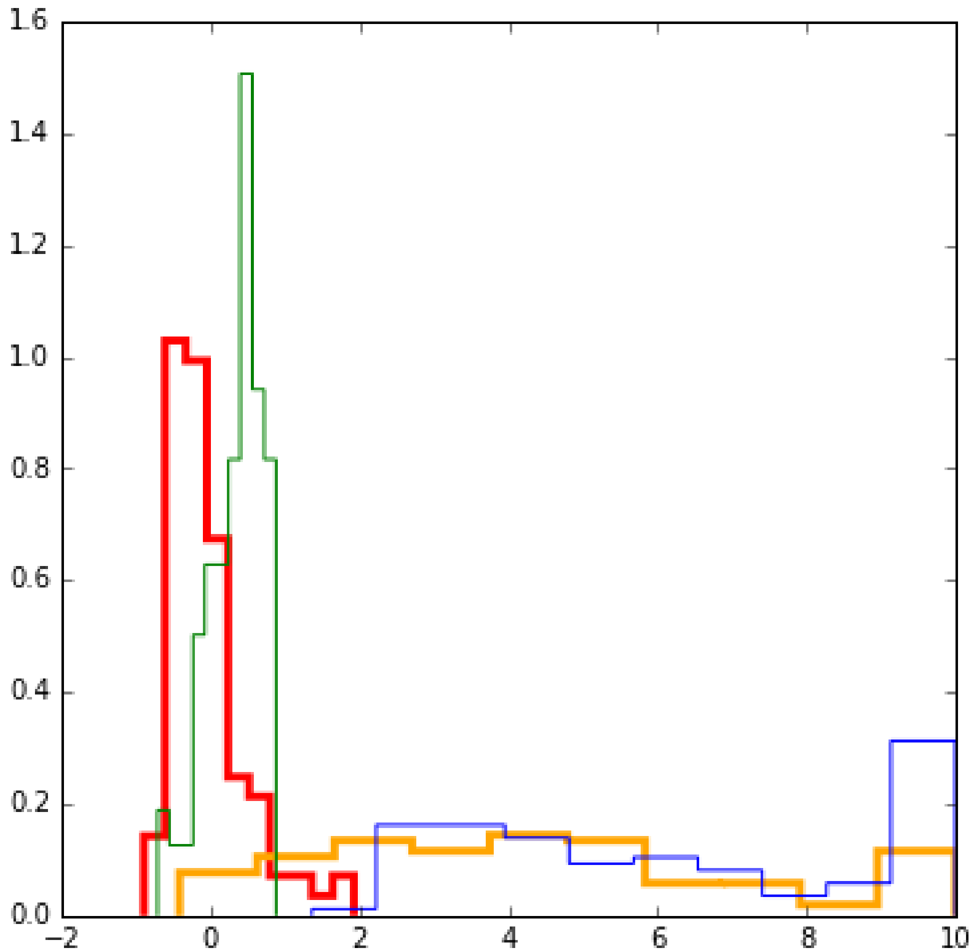
```
In [32]: # measures of non-Gaussianity: higher order moments

         def skew(v):
             return sqrt(len(v)) * sum((v-mean(v))**3) / sum((v-mean(v))**2)**1.5

         def excess_kurtosis(v):
             return len(v) * sum((v-mean(v))**4) / maximum(1e-5, sum((v-mean(v))**2)**2) - 3
```

```
In [33]: def feature_hist(features, kind=excess_kurtosis, xlog=False, maxk=10, **kw):
             data = array([kind(v) for v in features.T])
             if xlog: data = log10(maximum(1e-12, abs(data)))
             data = minimum(data, maxk)
             hist(data, **kw)
```

```
In [34]: # comparing input layer, PCA, and ICA

         feature_hist(nn100lin, histtype="step", color="red", normed=True, linewidth=3)
         feature_hist(nn100nonlin, histtype="step", color="orange", linewidth=3, normed=True)

         feature_hist(pca.transform(images), histtype="step", color="green", normed=True)
         feature_hist(ica.transform(images), histtype="step", color="blue", normed=True)
```



summary



The linear input layer generates distributions that are close to PCA distributions of non-Gaussianity.

After the non-linearity, we see non-Gaussian distributions in the neural network comparable to ICA.

7.5 PCA/ICA Input + Sigmoid + Output Layer

Since the input layer is so similar to a PCA transform, what happens if we actually replace it with PCA?

Since PCA isn't necessary "shifted" the right way relative to the nonlinearity, we add a BatchNorm1d layer, which learns a scale and bias separately for each feature.

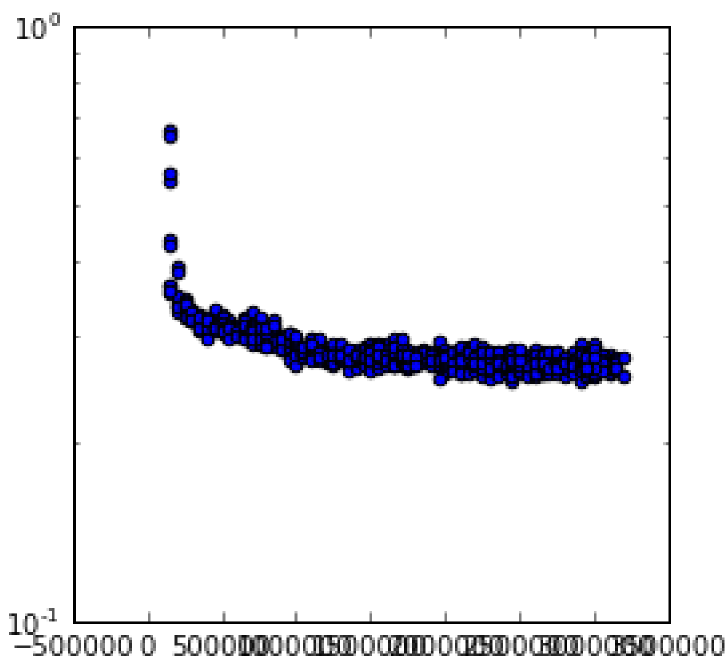
```
In [35]: pca = decomposition.PCA(100)
         pca.fit(images.reshape(len(images), -1))
         cupca = torch.FloatTensor(pca.transform(images)).cuda()
         cutest_pca = torch.FloatTensor(pca.transform(test_images)).cuda()
```

First, we explicitly transform the input images into PCA space.

```
In [36]: k = len(pca.components_)

         def make_model():
             return nn.Sequential(nn.BatchNorm1d(k),
                                  nn.Sigmoid(),
                                  nn.Linear(k, 10))
```

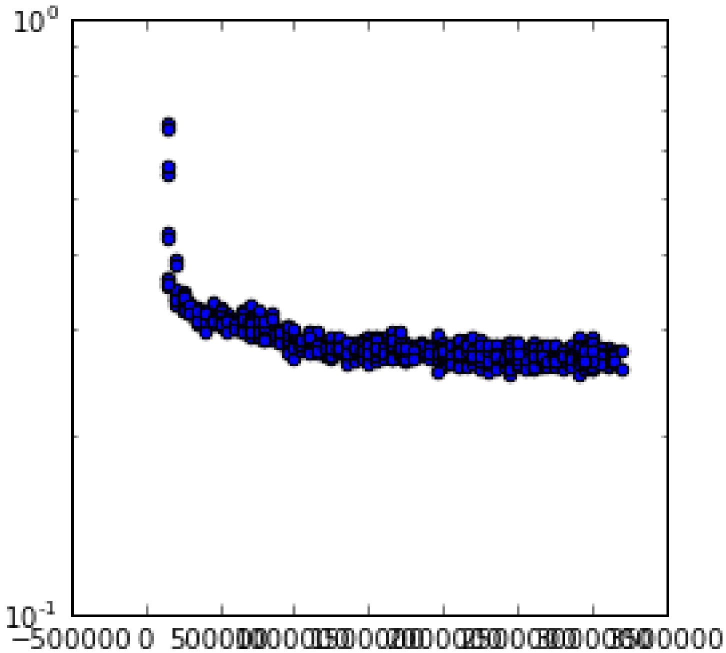
Next, we create a model that uses the PCA outputs as inputs. Since we don't know the absolute scale of the PCA components, we add a batch norm layer to linearly transform the activation of each component.

```
In [37]: amlp = imgclass.AutoMLP(make_model, cupca, cuclasses, cutest_pca, cutest_classes,
                                 initial_bs=500, maxtrain=5000000)
         nnpca = amlp.train()
         nnpca.cuda()
```



```
#best 0.0762 @ 3150000 of 3050000
```

```
Out[37]: Sequential(
           (0): BatchNorm1d(100, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
           (1): Sigmoid()
           (2): Linear(in_features=100, out_features=10, bias=True)
         )
```

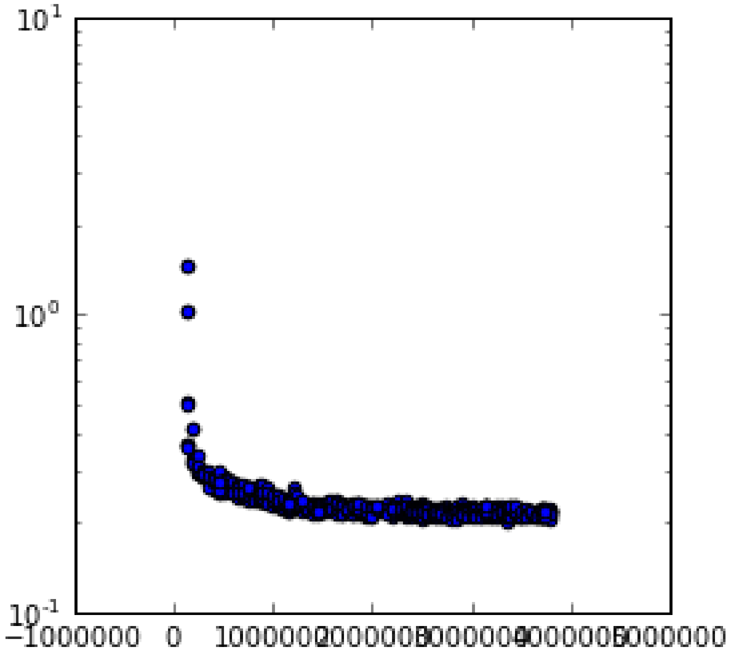



```
In [38]: cuica = torch.FloatTensor(ica.transform(images)).cuda()
         cutest_ica = torch.FloatTensor(ica.transform(test_images)).cuda()
```

Let's try the same with ICA.

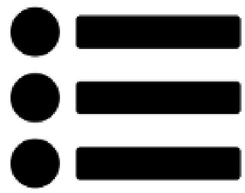
```
In [39]: k = len(ica.components_)

         def make_model():
             return nn.Sequential(nn.BatchNorm1d(k),
                                  nn.Sigmoid(),
                                  nn.Linear(k, 10))
```

```
In [40]: amlp = imgclass.AutoMLP(make_model, cuica, cuclasses, cutest_ica, cutest_classes,
                                 initial_bs=500, maxtrain=5000000)
         amlp.train()
```

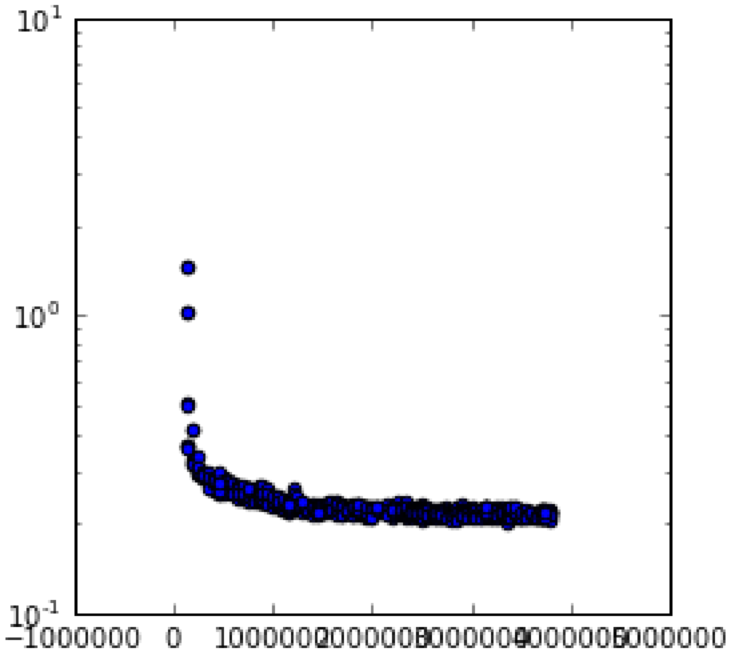



```
#best 0.0621 @ 2850000 of 3800000
```

```
Out[40]: Sequential(
           (0): BatchNorm1d(100, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)
           (1): Sigmoid()
           (2): Linear(in_features=100, out_features=10, bias=True)
         )
```



summary



Replacing the linear input layer with a "pretrained" PCA/ICA layer results in substantially worse performance.

This is also a common kind of experiment when grafting different neural networks together (e.g., using different pretrained input layers).

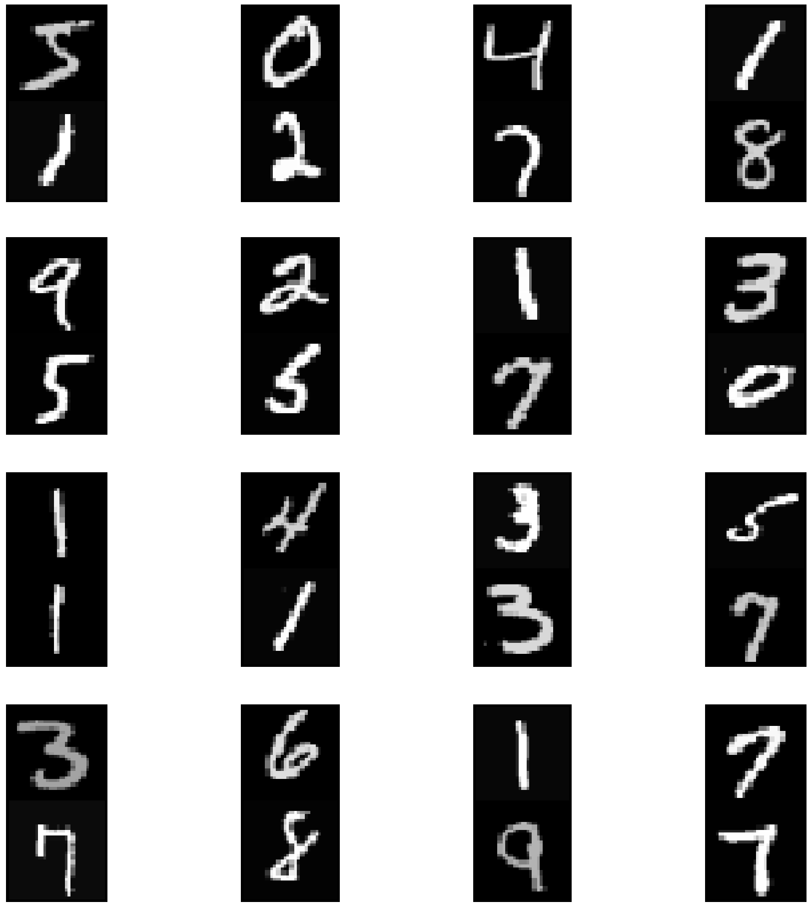
8 Irrelevant Features

Unsupervised: identify signal/noise by Gaussianity, magnitude.

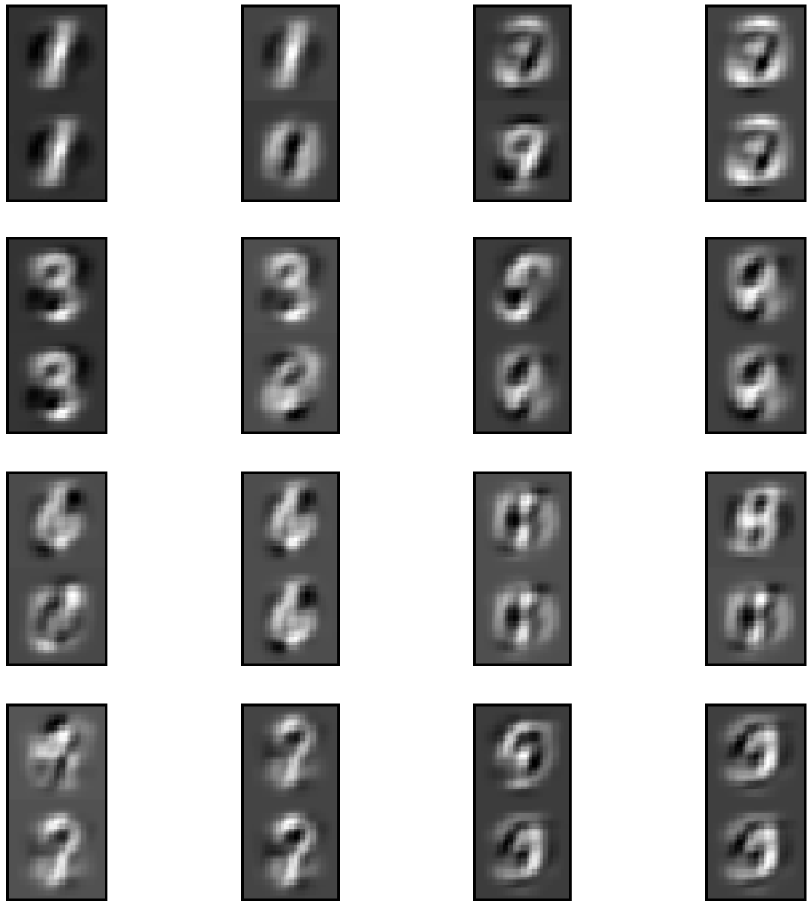
Supervised: identify signal/noise from backpropagated deltas?

```
In [41]: # Generate data with "noise": top half of image is relevant, bottom is not.

         perm = range(60000); random.shuffle(perm)
         pairs = hstack([images, images[perm,:]]).reshape(60000, 56*28)
         cupairs = torch.FloatTensor(pairs).cuda()
         perm = range(10000); random.shuffle(perm)
```

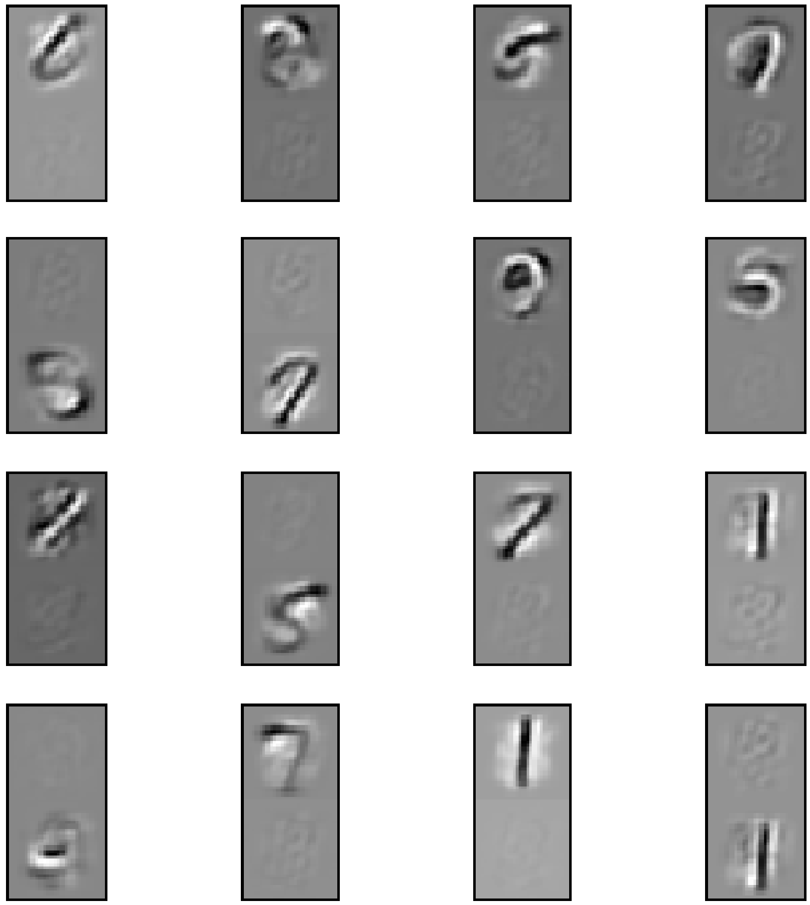
```
test_pairs = hstack([test_images, test_images[perm,:]]).reshape(10000, 56*28)
cutest_pairs = torch.FloatTensor(test_pairs).cuda()
showgrid(pairs.reshape(-1, 56, 28))
```



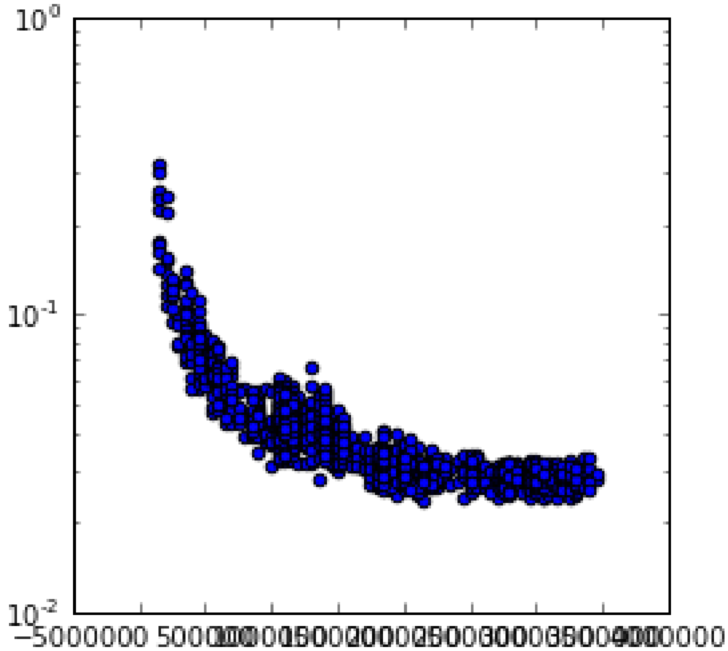
```
In [42]: # PCA mixes up top and bottom characters because it tries to find an optimal code in th

         k = 100
         pca = decomposition.PCA(k)
         pca.fit(pairs.reshape(len(pairs), -1))
         pca_basis = pca.inverse_transform(diag(ones(k))).reshape(k, 56, 28)
         showgrid(pca_basis)
```



In [43]:
```
# ICA recognizes the top and bottom components as "independent causes"
# and represents them as separate dimensions in ICA space, but can't determine relevanc

k = 100
ica = decomposition.FastICA(k)
ica.fit(pairs.reshape(len(pairs), -1))
ica_basis = ica.inverse_transform(diag(ones(k))).reshape(k, 56, 28)
showgrid(ica_basis)
```

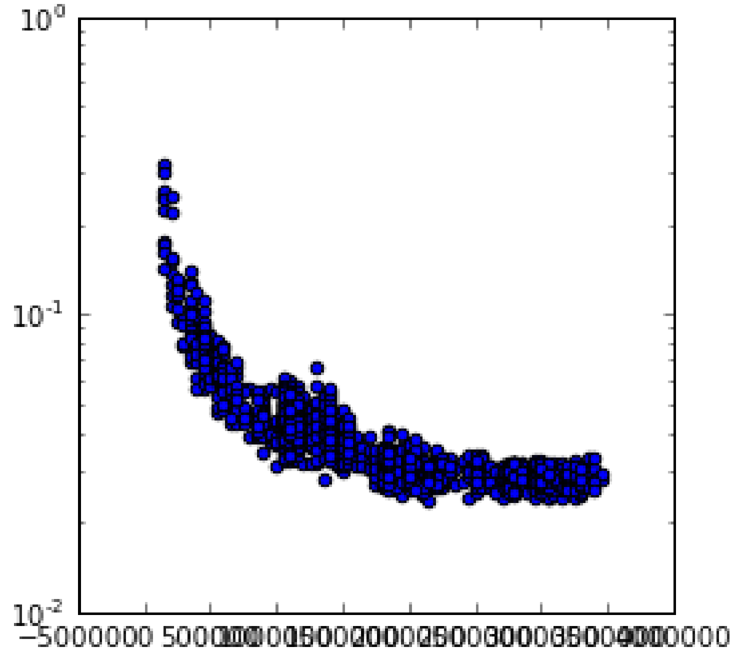


In [44]:
```
# train a network to perform classification

def make_model():
    return nn.Sequential(nn.Linear(56*28, 100), nn.Sigmoid(), nn.Linear(100, 10))

amlp = imgclass.AutoMLP(make_model, cupairs, cuclasses, cutest_pairs, cutest_classes,
                        initial_bs=20, maxtrain=10000000, decay=1e-5)
figsize(8, 8)
pnn100 = amlp.train()
pnn100.cuda()
```

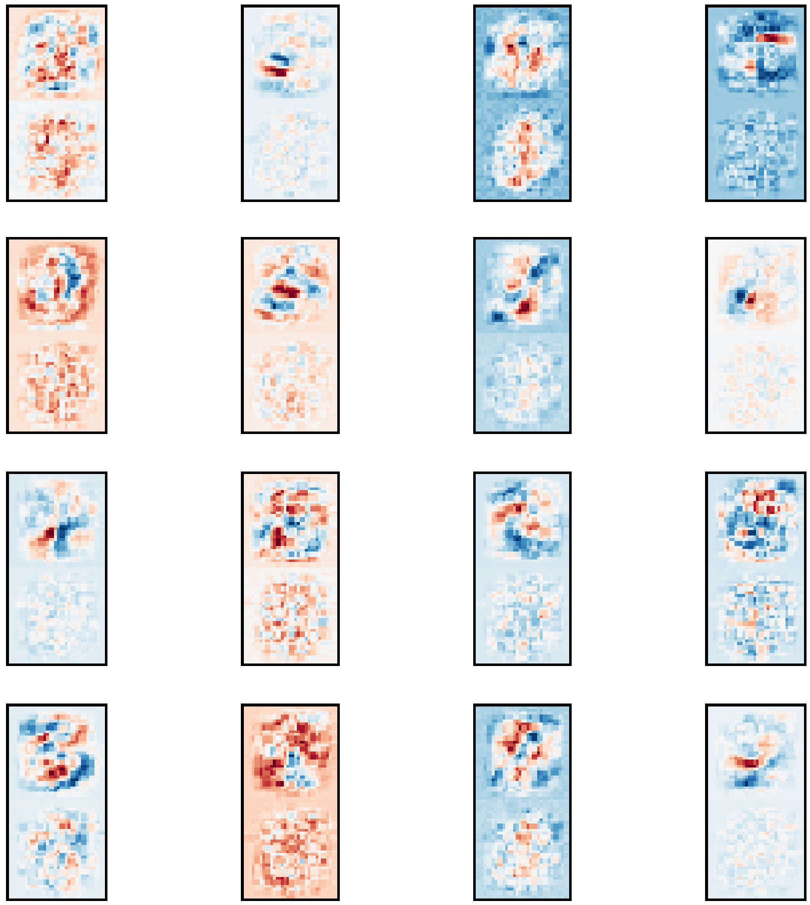



```
#best 0.0256 @ 2850000 of 3400000
```

```
Out[44]: Sequential(
           (0): Linear(in_features=1568, out_features=100, bias=True)
           (1): Sigmoid()
           (2): Linear(in_features=100, out_features=10, bias=True)
         )
```

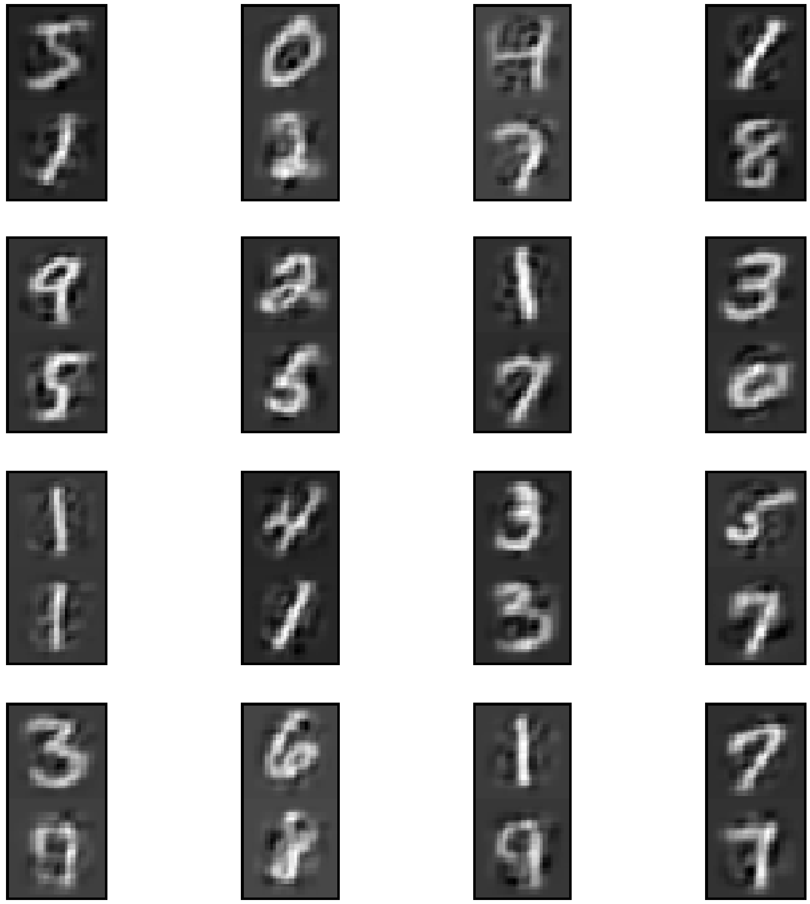


In [45]:
```
# display weights; note substantial non-zero weights in bottom half

W = N(pnn100[0].weight)
showgrid(W.reshape(100, 56, 28), cmap=cm.RdBu)
```



In [46]:
```
# weights are much larger at the top than at the bottom

pca = decomposition.PCA(20)
pca.fit(W.reshape(len(W), -1))
showgrid(pca.components_.reshape(-1, 56, 28), cmap=cm.RdBu)
```

In [47]:
```
# nevertheless, we can still reconstruct the full inputs from the linear subspace

pnn100first_layer = N(pnn100[0](cupairs))
pnn100recon = dot(pnn100first_layer, dot(pinv(pnn100first_layer), cupairs))
showgrid(pnn100recon.reshape(-1, 56, 28))
```

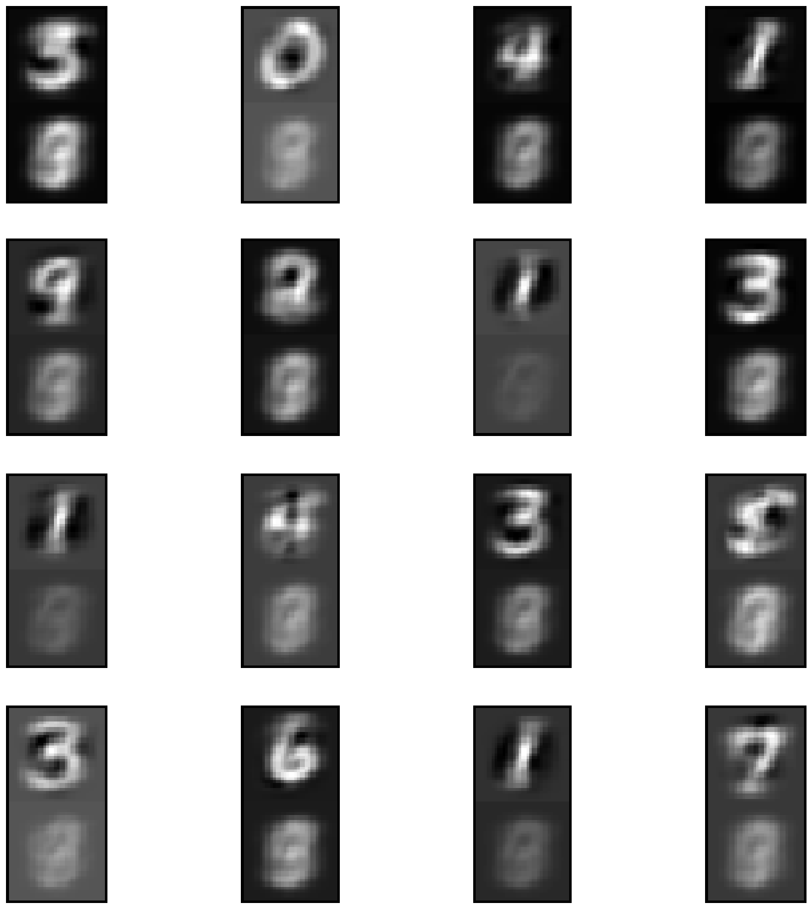


8.1 Why?

We are projecting a 784-dimensional space into 100-dimensional subspace.
Why is the information about the irrelevant features still recoverable after the linear projection?

```
In [48]: # after the nonlinearity, the information on the bottom half is largely destroyed,
         # and the top half becomes harder to decode linearly

         pnn100sig = N(nn.Sequential(*pnn100[:3])(cupairs))
         pnn100sigrecon = dot(pnn100sig, dot(pinv(pnn100sig), cupairs))
         showgrid(pnn100sigrecon.reshape(-1, 56, 28))
```

summary



Linear layers tend to have large weights for relevant features, small weights for irrelevant features.

Nevertheless, irrelevant information tends to be recoverable even after the linear layer.

It is the nonlinear layers that finally destroys the irrelevant information / noise.

9 Summary

9.1 Summary (Observations)

For fully connected layers with logistic hidden units: - linear layers are often PCA-like - information is destroyed in the non-linear layer

9.2 Summary (Techniques)

We have seen a number of useful experiments/tools:

- PCA, ICA, RICA, pseudo-inverse
- use measures of non-Gaussianity to determine whether layers aim for complete representation, non-Gaussianity, sparsity
- grafting together different networks
- techniques can be generalized by replacing linear methods with DNNs (at the cost of optimality)