Some Statistical Aspects of Photometric Redshift Estimation

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Photometric Redshift Estimation Background

Non–Negative Least Squares

Non–Negative Matrix Factorization

EAZY Results

Outline

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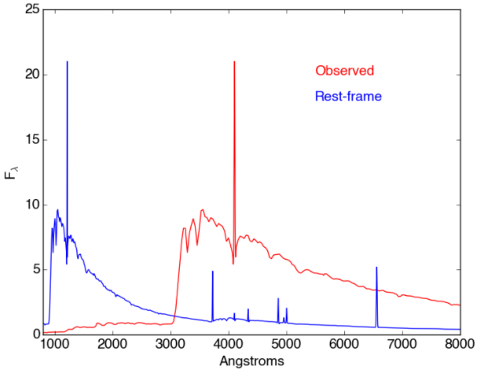
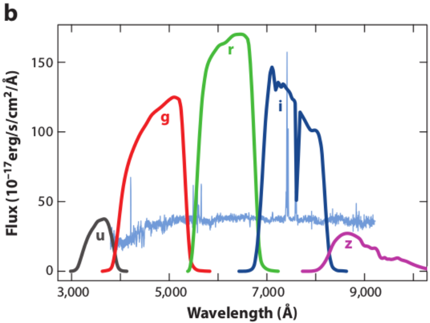
Redshift



- f_{obs} (red line) is the observed spectrum
- f_{rf} (blue line) is the true, unobserved spectrum
- $f_{rf}(\lambda) = f_{obs}(\lambda(1 + z))$
- goal: estimate z
- relatively easy if we observe f_{obs}

Photometric Data

- spectral data is very expensive to collect
- much more photometric data available
- photometry is the spectra observed at small set of wavelengths



Photometric redshift estimation (photoz) is the process of estimating redshift from photometric data.

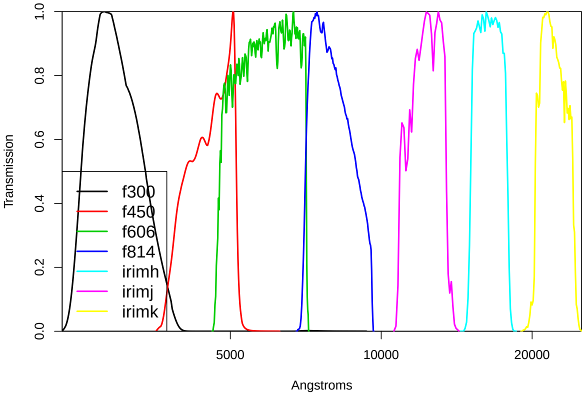
Source: Schafer "A Framework for Statistical Inference in Astrophysics."
`http://www.annualreviews.org/doi/abs/10.1146/annurev-statistics-022513-115538`

Machine Learning Approach to Photoz

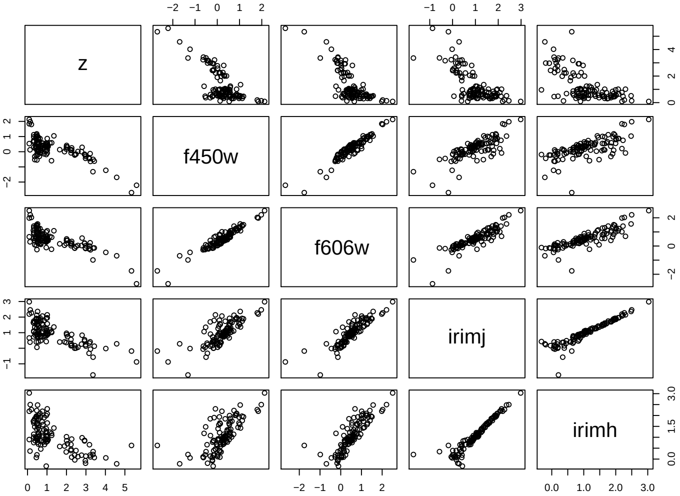
Idea:

- create training set by taking spectroscopy on subset of data
- construct classifier on training data, apply to unlabeled data

Example: Collected photometry in 7 filters for 114 galaxies.

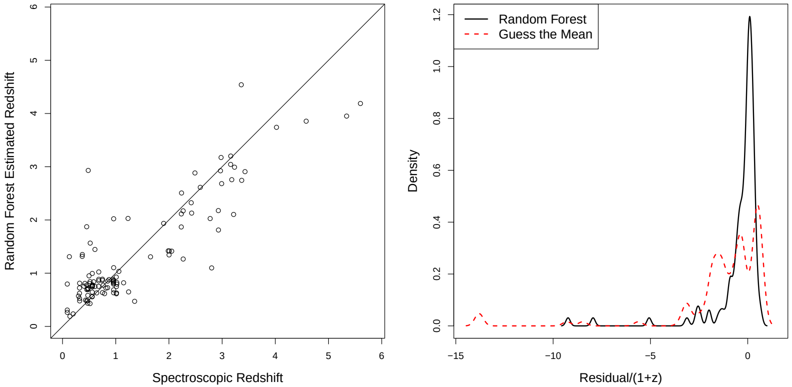


Spectroscopic Redshift and Photometry



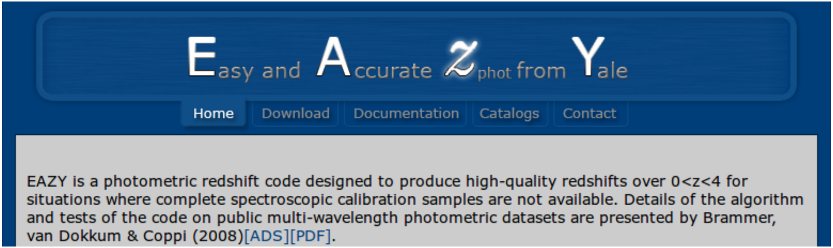
Only showing 4 of 7 filters.

Apply Random Forest



- ignored uncertainty in photometry (features)
- training sets are often from nearby objects, unlabeled data far away objects
- difficult to compute uncertainty in estimate

Easy Accurate Zphot from Yale (EAZY)



- developed by Brammer, van Dokkum, Coppi
- synthesizes ideas from several earlier works

Paper: http://adsabs.harvard.edu/abs/2008ApJ...686.1503B. Code: https://github.com/gbrammer/eazy-photoz/

Simple Idea

Notation:

- determine set of model spectra T_i for $i = 1, \ldots, n_T$
  - actual spectra
  - spectra generated by theoretical models
- let $T_{z,i}$ be spectra i redshifted to z
- let $T_{j,z,i}$ be spectra i redshifted to z, convolved with filter j
- F_j and σ_j are the flux and flux error in band j

Optimization Function:

$$\widehat{z} = \underset{z}{\operatorname{argmin}} \min_{1 \leq i \leq n_T} \sum_{j=1}^{J} \left(\frac{T_{j,z,i} - F_j}{\sigma_j} \right)^2$$

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Generalizing the Template Set

Consider expanding templates through linear combinations

$$T_z = \sum_{i=1}^{n_T} \alpha_i T_{z,i} = \boldsymbol{\alpha}^T T_z$$

Astronomical theory says that $\alpha_i \geq 0 \ \ \forall i$. So optimization problem becomes

$$\widehat{z} = \underset{z}{\operatorname{argmin}} \ \min_{\boldsymbol{\alpha}:\boldsymbol{\alpha}>0} \sum_{j=1}^{J} \left(\frac{\boldsymbol{\alpha}^T T_z - F_j}{\sigma_j} \right)^2$$

This is known as non–negative least squares in statistics.
Solve on a grid of z.

More Familiar Statistical Notation

The non-negative least squares estimate is

$$\widehat{\beta} = \underset{\beta:\beta\geq 0}{\text{argmin}}\ ||Y - X\beta||_2^2$$

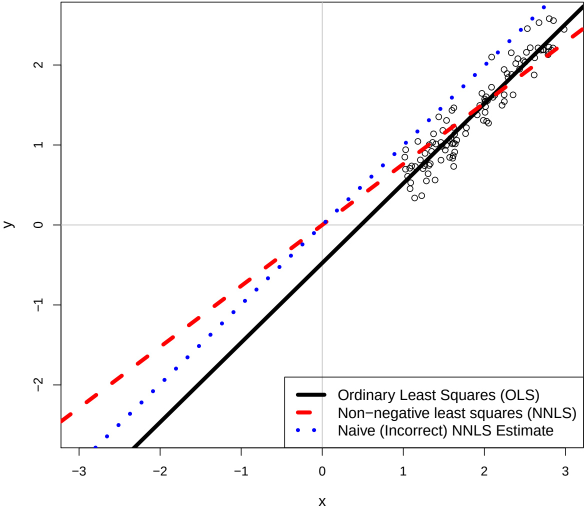
where

- $X \in \mathbb{R}^{n \times p}$ is design matrix
- $Y \in \mathbb{R}^{n}$ is response

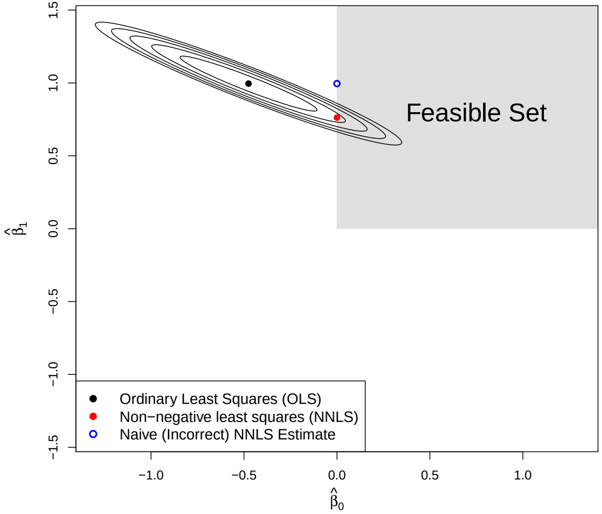
without the $\beta \geq 0$ constraint the problem has the familiar LS form

$$\underset{\beta}{\text{argmin}}\ ||Y - X\beta||_2^2 = (X^T X)^{-1} X^T Y.$$

Example Data



Example Likelihood Surface



Non–Negative Least Squares Algorithms

- `R`–package `nnls` and `scipy.optimize.nnls` use active set method (Lawson and Hanson 1974 book "Solving Least Squares Problems")
- EAZY uses "Multiplicative Updates for Nonnegative Quadratic Programming" by Sha 2007 *Neural Computation*

Outline

Constructing Template Set

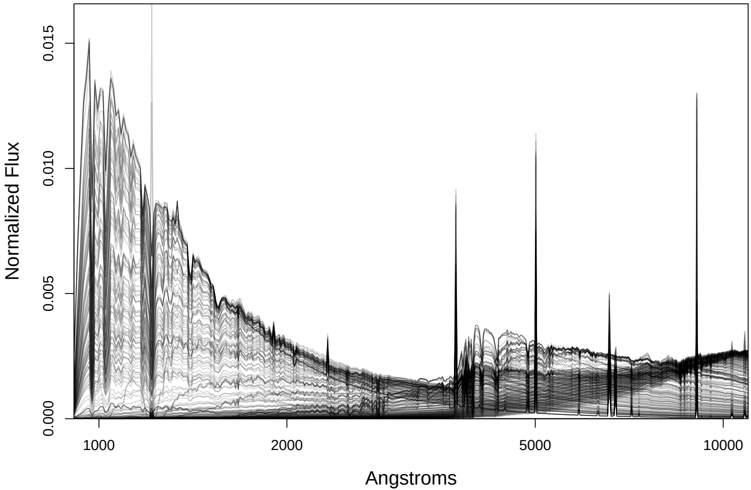
T_i are the templates. They may be

- observed data
  - advantages: "real" data that does not make physical assumptions
  - disadvantages: sometimes expensive to collect, little data available at high redshifts
- output from physical simulations
  - advantages / disadvantages reversed from observed data

Having a small set of T_i is convenient because

- interpretation is easier
- computation is faster

Constructing Template Set



T_i for $i = 1, \ldots, 259$ filters, lots of redundancy, like to reduce set

Dimension Reduction for Template Construction

- $X \in \mathbb{R}^{n \times p}$ are templates
  - $n =$ number of templates
  - $p =$ number of bins for each tempate
- p is the "dimension" of the data
- assume: the row vectors x_i are (approximately) in some lower dimensional subspace of $\mathbb{R}^p$
- finding and characterizing this subspace is called "dimension reduction"

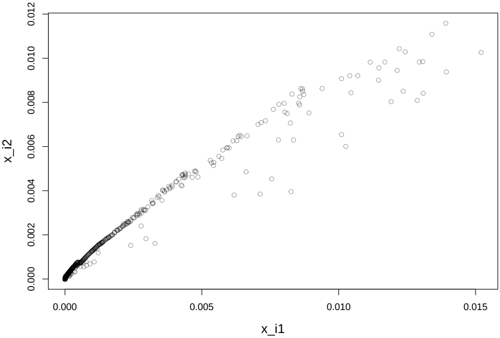
We would like this subspace to be characterized as a linear combination of <u>positive</u> bases.

Dimension Reduction Example

consider

$$\{(x_{i1}, x_{i2})\}_{i=1}^{n}$$

the first two dimensions of filters



Message:

- intrinsic dimension is near 1
- can compress the two dimensional data into 1 dimension

Principal Components Analysis (PCA) Idea

- realign axes so
  - most variation on first axis
  - second most variation on second axis
  - ...
- ignore higher axes because minimal variation in these directions
- principal components describe how the new axes map to the old axis

PCA is typically applied to a scaled version of X.

$$X^* = (X - 1\mu^T)S^{-1}$$

- remove column means (μ)
- scale column variances to 1
  - S is diagonal with S_{jj} = standard deviation column j of X

PCA Math – Singular Value Decomposition

The singular value decomposition of X^* (assuming $n > p$) is

$$X^* = U\Sigma V^T$$

where

- U is $n \times p$ with $U^T U = I$[1]
  - data in the new coordinate system.
- V is $p \times p$ with $V^T V = I$
  - V rotates the new coordinates to the old coordinates.
- Σ is $p \times p$ diagonal with $\Sigma_{jj} > \Sigma_{ii}$ for $j < i$ [2]
  - Σ scales the new coordinates to the old coordinates.

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[1] U is $n \times p$ in R and $n \times n$ in theory.

[2] Σ is $p \times p$ in R and $n \times p$ in theory.

Reconstructing the data

- a $q \leq p$ dimensional reconstruction of X^* (in R notation) is

$$X_q^* = U[,1{:}q]\Sigma[1{:}q, 1{:}q]V[,1{:}q]^T$$

- if the data lies (approximately) on a q dimensional subspace then

$$X^* \approx X_q^*$$

- obtain an approximation of the original data

$$X_q = X_q^* S + 1\mu^T$$

and

$$X \approx X_q$$

- reduced template set is $V[,1{:}q]$

Non–negative Matrix Factorization

Decomposition: When the data matrix X is positive we can decompose

$$X_{n \times p} \approx W_{n \times r} H_{r \times p}$$

where rows of H are basis.

Algorithm: Maximize

$$L(W, H) = \sum_{i=1}^{n} \sum_{j=1}^{p} (x_{ij} \log(WH)_{ij} - (WH)_{ij})$$

ie maximum likelihood under the model that x_{ij} is Poisson$((WH)_{ij})$

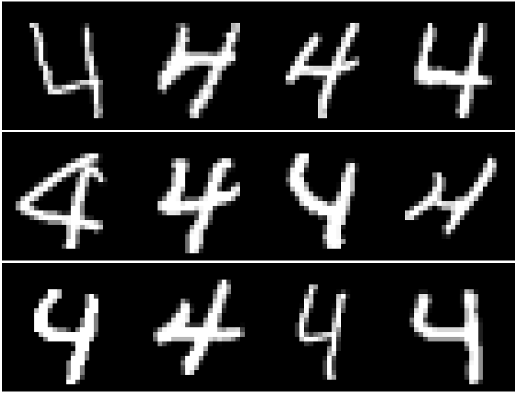
Source: Elements of Statistical Learning. Haste, Tibshirani, Friedman. Chapter 14.6. Available: `http://statweb.stanford.edu/~tibs/ElemStatLearn/`

Non–negative Matrix (NMF) Factorization

- the NMF basis vectors often have more physical interpretation than PCA basis
  - eg NMF spectral basis elements look like spectra
- optimizing log likelihood difficult for NMF
- identifiability issues with model*

Source: Donoho and Stodden. "When Does Non-Negative Matrix Factorization Give a Correct Decomposition into Parts?"
https://web.stanford.edu/~vcs/papers/NMFCDP.pdf

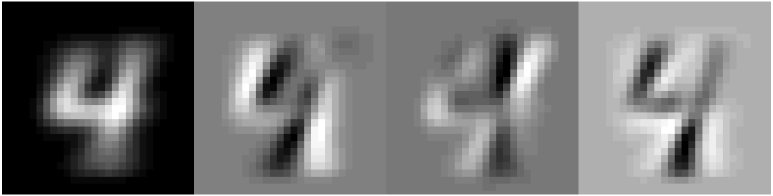
MNIST Data Set – 12 Fours Out of 4072



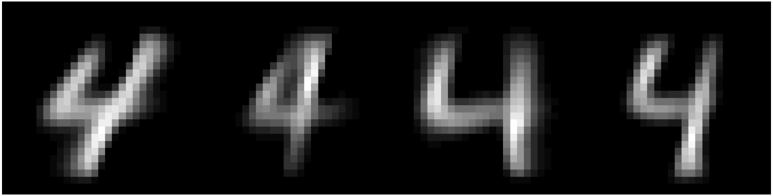
- each image 28×28 pixels
- vectorize image i to $x_i \in \mathbb{R}^{784}$
- $X \in \mathbb{R}^{4072 \times 784}$
- apply PCA and NMF

MNIST Results PCA versus NMF

PCA (Mean + 3 principal components)



NMF (4 Basis Vectors)



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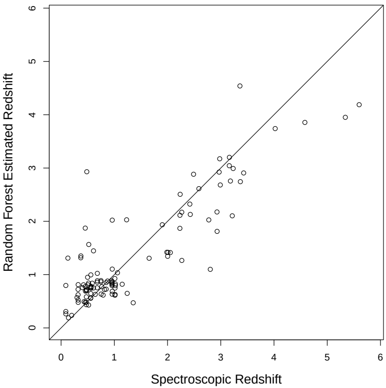
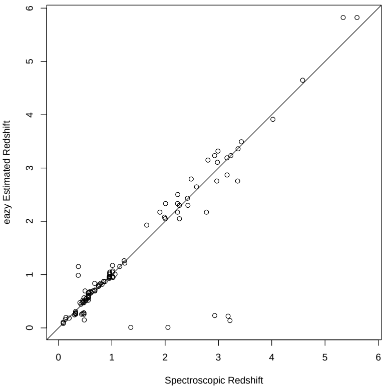
Random Forest – EAZY Comparison





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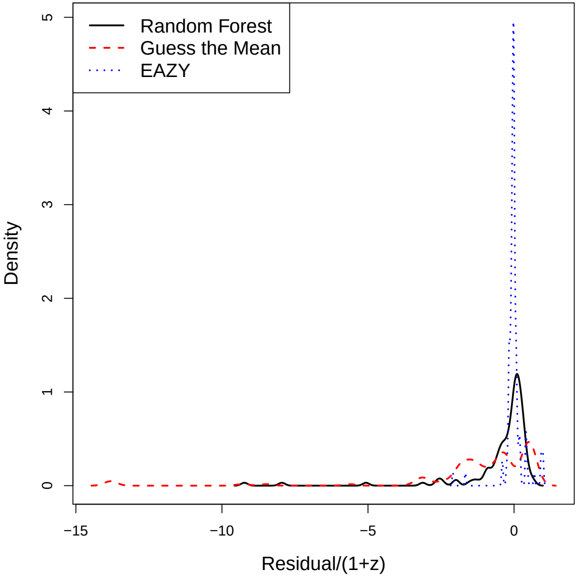

Other Challenges / Opportunities / Approaches

- accounting for template error (model misspecification)
- estimating templates from photometric data
- propagating uncertainty on redshift to the next stage of analysis
- other work on photoz:
  - "Robust machine learning applied to astronomical data sets. III. Probabilistic photometric redshifts for galaxies and quasars in the SDSS and GALEX." Ball ApJ 2008
  - "Bayesian photometric redshift estimation." Benitez ApJ 2000
  - "Random forests for photometric redshifts." Carliles ApJ 2010