

PRINCIPAL COMPONENT ANALYSIS OF SLOAN DIGITAL SKY SURVEY STELLAR SPECTRA

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ABSTRACT

We apply Principal Component Analysis (PCA) to $\sim 100,000$ stellar spectra obtained by the Sloan Digital Sky Survey (SDSS). In order to avoid strong nonlinear variation of spectra with effective temperature, the sample is binned into 0.02 mag wide intervals of the $g-r$ color ($-0.20 < g-r < 0.90$, roughly corresponding to MK spectral types A3–K3), and PCA is applied independently for each bin. In each color bin, the first four eigenspectra are sufficient to describe the observed spectra within the measurement noise. We discuss correlations of eigencoef-ficients with metallicity and gravity estimated by the Sloan Extension for Galactic Understanding and Exploration Stellar Parameters Pipeline. The resulting high signal-to-noise mean spectra and the other three eigenspectra are made publicly available. These data can be used to generate high-quality spectra for an arbitrary combination of effective temperature, metallicity, and gravity within the parameter space probed by the SDSS. The SDSS stellar spectroscopic database and the PCA results presented here offer a convenient method to classify new spectra, to search for unusual spectra, to train various spectral classification methods, and to synthesize accurate colors in arbitrary optical bandpasses.

Key words: methods: data analysis – stars: abundances – stars: fundamental parameters – stars: statistics

Online-only material: color figures

1. INTRODUCTION

A large number of homogeneously obtained stellar spectra have recently become available. For example, the Sloan Digital Sky Survey (SDSS; York et al. 2000) has made publicly available¹ over 460,000 stellar spectra as a part of its Data Release 7 (Abazajian et al. 2009), and Radial Velocity Experiments² (RAVE) may provide up to a million spectra over the next few years. This rapid progress in the availability of stellar spectra re-opens the old question of optimal stellar parameter extraction. For example, the SDSS estimates effective temperature, gravity, and metallicity using a variety of standard methods implemented in an automated pipeline (Sloan Extension for Galactic Understanding and Exploration Stellar Parameters Pipeline, hereafter SSPP; Beers et al. 2006). A detailed discussion of these methods and their performance can be found in Allende Prieto et al. (2006, 2008) and Lee et al. (2008a, 2008b). The results of different methods implemented in the SSPP are *averaged* to obtain the final adopted values in the SDSS Spectral Parameter Pipeline table (*sppParams*). Although a detailed analysis by Lee et al. (2008a, 2008b) demonstrates that systematic metallicity differences between the methods used in averaging do not exceed ~ 0.1 dex (with random errors in the range 0.1–0.3 dex), it is fair to ask whether a single method could be used to obtain the same level of systematic and random errors, instead of combining different methods with varying error properties.

Principal Component Analysis (PCA) has been demonstrated as a viable tool in solving this classification problem (Connolly et al. 1995; Connolly & Szalay 1998; Bailer-Jones et al. 1998; and references therein). Yip et al. (2004) have developed a PCA-based analysis code specialized to SDSS spectra. Here, we use the same code to investigate whether the PCA eigencoef-ficients (ECs) are correlated with the metallicity and gravity obtained

by the SSPP. Byproducts of this analysis are high signal-to-noise eigenspectra that can be used to generate spectra for any combination of basic stellar parameters (effective temperature, metallicity, and gravity) within the parameter space probed by SDSS. Hence, given an arbitrary spectrum, one can attempt a low-dimensional fit using our library of eigenspectra. Among numerous drivers for such a library, we single out a photometric calibration scheme for the Large Synoptic Survey Telescope (LSST).³ LSST plans to use an auxiliary spectroscopic telescope to obtain spectra of standard stars at the same time as the main imaging survey is performed (see Ivezić et al. 2008a). The atmospheric transmission properties, required to photometrically calibrate the imaging survey, will be obtained by simultaneously fitting the stellar spectrum and a sophisticated atmospheric model with six free parameters for each observation. The ability to describe the expected stellar spectra in a low-dimensional continuous space by using a small number of eigenvectors, with ECs that are not defined on a fixed grid, might increase the fidelity of the fitted model.

In Section 2, we describe our sample selection and the application of PCA to SDSS stellar spectra. We discuss our results in Section 3, and end with a summary in Section 4.

2. PRINCIPAL COMPONENT DECOMPOSITION OF SDSS STELLAR SPECTRA

2.1. The Properties of SDSS Spectra

In addition to massive amounts of optical photometry of unprecedented quality, the SDSS has also produced a large spectroscopic database. A compendium of technical details about SDSS can be found on the SDSS web site,⁴ which also provides an interface for public data access. Targets for the spectroscopic survey are chosen from the SDSS imaging data based on their colors and morphological properties (Strauss

¹ See <http://www.sdss.org/dr7>

² See <http://www.rave-survey.aip.de/rave>

³ See <http://www.lsst.org/>

⁴ See <http://www.sdss.org/>

et al. 2002; Eisenstein et al. 2001; Richards et al. 2002). In the spectroscopic survey, stars are targeted either as calibrators or for scientific reasons in specific parts of the four-dimensional SDSS color space (Yanny et al. 2009).

A pair of multi-object fiber-fed spectrographs mounted onto the SDSS 2.5 m telescope (Gunn et al. 2006) is used to take 640 simultaneous spectra within a radius of 1.49° , each with a wavelength coverage of 3800–9200 Å and a spectral resolution of ~ 2000 , and with a signal-to-noise ratio of >4 per pixel at $g = 20.2$. Spectro-photometric calibration of these spectra is exquisite; for example, the imaging magnitudes and the stellar magnitudes synthesized from SDSS spectra agree with an rms of only ~ 0.05 mag (see Smolčić et al. 2004).

2.2. Sample Selection

We begin by selecting bright stars in SDSS Data Release 6 that have colors consistent with the main stellar locus (Lenz et al. 1998; Fan 1999; Finlator et al. 2000), or are found in the regions populated by RR Lyrae stars (Ivezić et al. 2005) and blue horizontal branch stars (Sirko et al. 2004). Stars that are probable white dwarf–red dwarf pairs (Smolčić et al. 2004) or single hot white dwarfs (Eisenstein et al. 2006) are not selected. We only use stars from the sky regions with modest interstellar dust extinction, determined using the interstellar dust maps of Schlegel et al. (1998).

The specific criteria applied to 130,620 entries from the SDSS DR6 version of *sppParams* table⁵ that have $\log(g) > 0$ are the following (the number in brackets indicates the number of stars remaining after each selection step):

1. The interstellar extinction in the r band below 0.3; [106,816].
2. $14 < g < 19.5$; [104,844].
3. $-0.2 < g - r < 0.9$; [103,588].
4. $0.7 < u - g < 2.4$; [101,630].
5. $\{-0.2 < g - r - 0.5(u - g - 0.5) < 0.4\}$ OR $\{u - g < 1.4$ AND $g - r < 0.25\}$; [100,759].
6. $-0.2 < 0.35(g - r) - (r - i) < 0.20$; [98,063].

For each star, the data analyzed in this work include the *ugriz* photometry, SDSS spectrum, and SSPP estimates of effective temperature (T_{eff}), metallicity ($[\text{Fe}/\text{H}]$), and gravity ($\log(g)$). The selected stars span the range of effective temperature from ~ 4500 K to ~ 9000 K (see below), and 99.4% have metallicity in the range $-3 < [\text{Fe}/\text{H}] < 0$ with a median of -1.0 . While the sample is dominated by main-sequence stars (the median $\log(g)$ is 4.1 ± 0.44 dex), a small fraction of stars ($\sim 3\%$) have lower gravity estimates consistent with giants (see Figure 1).

2.3. The $g - r$ Color Binning

Stellar spectra are to the zeroth order similar to the Planck (blackbody) function controlled by the effective temperature; however, their variations of spectral line width and strength depend not only on effective temperature but also on metallicity and gravity. At a chosen effective temperature, the metallicity affects the strength of the spectral line and gravity can broaden or narrow the spectral line. In order to study these variations due to metallicity and gravity at a given effective temperature, we group the stars with SDSS spectra into 55 color bins with a width of 0.02 mag, in the range $-0.2 < g - r < 0.9$. As shown by Ivezić et al. (2008b), this color is strongly correlated with the effective temperature determined by the SSPP: a 0.02 mag wide bin in the $g - r$ color roughly corresponds to one MK spectral

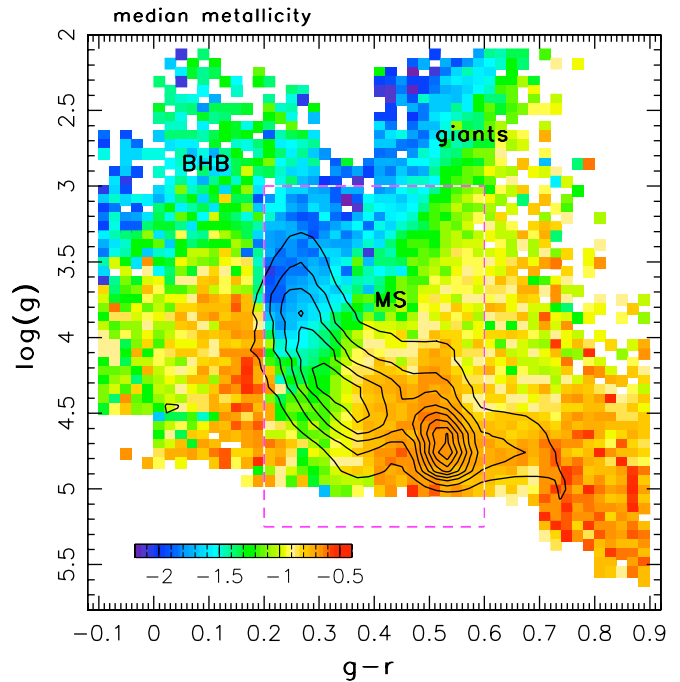


Figure 1. Linearly spaced contours show the distribution of $\sim 100,000$ stars with $g < 19.5$ from the SDSS DR6 spectroscopic sample in the $\log(g)$ vs. $g - r$ plane. The multi-modal distribution is a result of the SDSS target selection algorithm. The color scheme shows the median metallicity in all 0.02 mag by 0.06 dex large pixels that contain at least 10 stars (according to the legend shown in the bottom left corner). The fraction of stars with $\log(g) < 3$ (giants) is 4%, and they are mostly found in two color regions: $-0.1 < g - r < 0.2$ (blue horizontal branch stars) and $0.4 < g - r < 0.65$ (red giants). They are dominated by low-metallicity stars ($[\text{Fe}/\text{H}] < -1$). The dashed lines roughly outline the main-sequence (MS) region; see Ivezić et al. (2008b).

subtype. The best-fit expression derived by Ivezić et al. (2008b),

$$\log(T_{\text{eff}}/\text{K}) = 3.882 - 0.316(g - r) + 0.0488(g - r)^2 + 0.0283(g - r)^3, \quad (1)$$

achieves systematic errors below 0.004 dex and overall rms of 0.008 dex, within the $-0.3 < g - r < 1.3$ color range. The temperature range corresponding to the $g - r$ limits adopted here ($-0.2 < g - r < 0.9$) is 4550 K–8850 K. The number of stars per $g - r$ bin ranges from 430 to 9104, with a median of 1571. The variation of the number of stars in a bin, the median apparent magnitude, metallicity, gravity, and the fractions of low-metallicity stars ($[\text{Fe}/\text{H}] < -1$) and giants ($\log(g) < 3$) are shown in Figure 2.

Most of the stars in our sample are main-sequence stars with $\log(g) > 3$ and $[\text{Fe}/\text{H}] > -1$. The impact of metallicity and gravity on stellar spectra, as well as the fraction of stars in the sample that are not main-sequence disk stars, varies with effective temperature, i.e., with the $g - r$ color. For the purposes of presentation, we single out two bins in $g - r$. For the 4556 stars in bin 23 ($0.24 < g - r < 0.26$), we expect a strong correlation between the $u - g$ color and metallicity, as discussed in detail by Ivezić et al. (2008b). We use this bin to compare the random errors for metallicity estimates obtained from the SSPP and obtained here using PCA. For bin 37, with $0.52 < g - r < 0.54$ and 5195 stars, the fraction of giants is near its maximum ($\sim 10\%$). This bin enables a study of correlations between $\log(g)$ and PCA ECs. The color range of bin 37 was deliberately targeted for SDSS spectroscopy because giant stars are good probes of distant halo structure. The distribution of

⁵ See <http://www.sdss.org/dr6/products/spectra/spectroparameters.html>

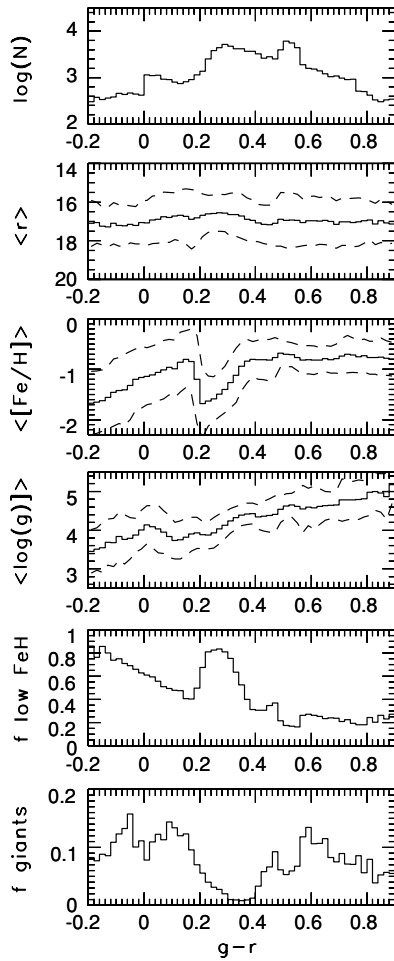


Figure 2. Top to bottom: solid lines show the variation of the number of stars in a given $g-r$ bin, the median apparent r -band magnitude, metallicity, gravity, and the fraction of low-metallicity stars ($[\text{Fe}/\text{H}] < -1$) and giants ($\log(g) < 3$). Dashed lines show the 1σ envelope around the medians. Stars with $g-r > 0.2$ are dominated by main-sequence stars, and the bluer stars are dominated by blue horizontal branch stars, RR Lyrae stars, and blue stragglers. The approximate $g-r$ colors for several MK spectral types (luminosity class V) are taken from Covey et al. (2007).

stars from these two bins in the $\log(g)$ versus $[\text{Fe}/\text{H}]$ metallicity diagram is compared to the full sample in Figure 3.

2.4. Principal Components Decomposition

For a thorough discussion of PCA and several of its various applications, we refer the reader to Connolly et al. (1995) and Yip et al. (2004). Briefly, PCA calculates eigenspectra, or characteristic averaged spectral shapes, from the input batch of spectra, and measures ECs that represent how strongly each eigenspectrum is present in a data spectrum. The PCA package we used was specifically developed for use with SDSS spectra (Yip et al. 2004). Before PCA decomposition occurs, the package shifts the spectra to their rest frames (zero radial velocity) and rebins them to a common wavelength range. The spectra are then repaired in gappy regions (i.e., bad pixels or missing data) using the iterative KL-correction formalism developed by Connolly & Szalay (1999). The PCA code outputs eigenspectra, ECs, and repaired data spectra.

We investigated spectral decompositions using varying numbers of eigenspectra and found that the first four eigencomponents are sufficient to describe the observed spectra within the measurement noise (for a single spectrum). Figure 4 compares

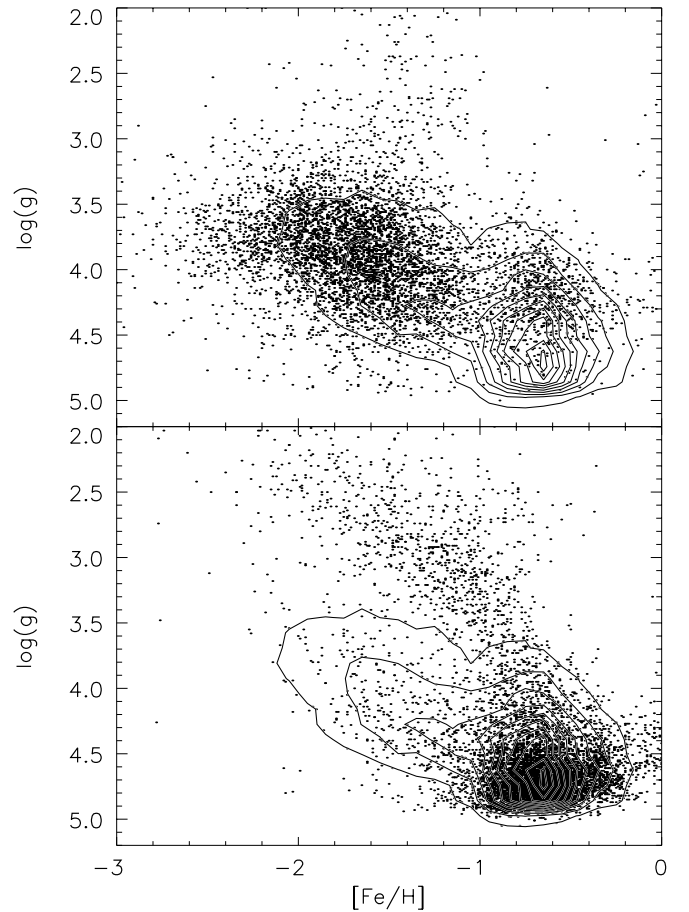


Figure 3. Bivariate metallicity–gravity distribution for two color bins. In both panels, the linearly spaced contours show the $\log(g)$ vs. $[\text{Fe}/\text{H}]$ distribution of the $\sim 100,000$ stars in the analyzed sample. The symbols in the top panel show stars from bin 23, and the bottom panel shows stars from bin 37. Bin 37 ($\log(g) < 3.5$ and $[\text{Fe}/\text{H}] < -1$) contains many low-metallicity giant stars.

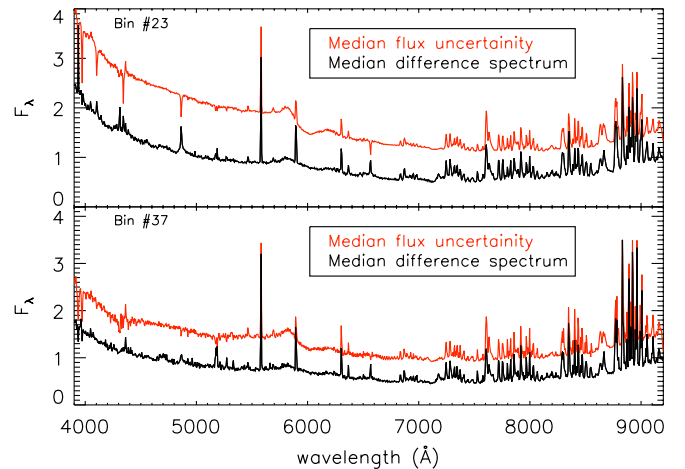


Figure 4. Median difference spectra and median noise spectra for bins 23 (top) and 37 (bottom). The median difference spectra are black and the median noise spectra are red. The median difference spectra were constructed by taking the absolute value of the difference of each original spectrum and its reconstructed spectrum and then taking the median of the difference spectra in vacuum wavelength bins of width 5 \AA . We took the median of the noise spectra in similar wavelength bins to create the median noise spectra. We demonstrate in both bins that the use of four ECs reconstructs the original spectra to within the measurement noise.

(A color version of this figure is available in the online journal.)

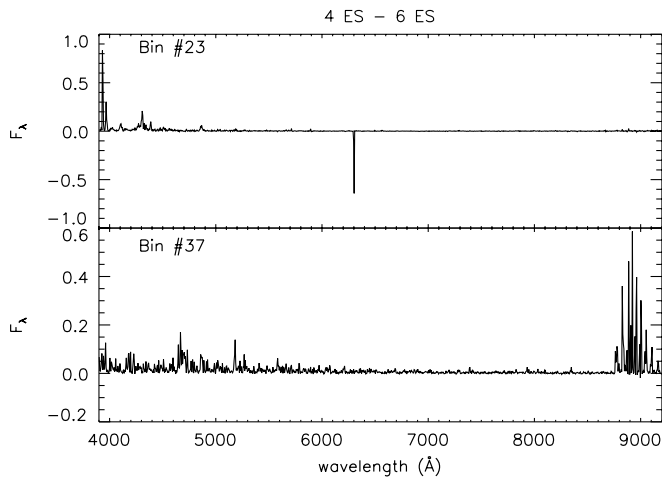


Figure 5. Comparison of the median difference spectra for PCA decompositions based on four and six eigenspectra for bins 23 (top) and 37 (bottom). The median difference spectra were constructed by taking the absolute value of the difference of each original spectrum and its reconstructed spectrum and then taking the median. The results for PCA decomposition based on four eigenspectra are shown in Figure 4. These two panels show the difference between the results from Figure 4 and analogous median difference spectra for six eigencomponents.

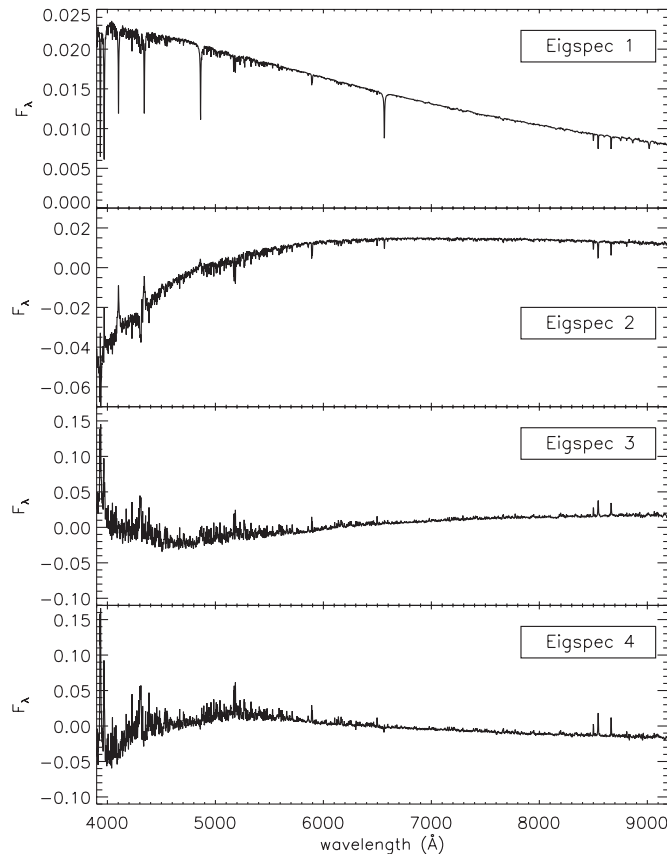


Figure 6. Four eigenspectra (F_λ) generated for the 4556 stars in bin 23 ($0.24 < g - r < 0.26$), plotted at vacuum wavelengths. The first eigenspectrum closely resembles a metal-poor ($[\text{Fe}/\text{H}] \sim -1.5$) subdwarf. The variation of spectra in this bin is expected to be dominated by the variation of stellar metallicity.

the median difference between the original and reconstructed spectra with the median noise in the original spectra for bins 23 and 37. As shown, the spectra reconstructed using four eigencomponents are consistent with the original spectra to well within the typical measurement error. Furthermore, Figure 5 demonstrates that the difference between PCA decompositions

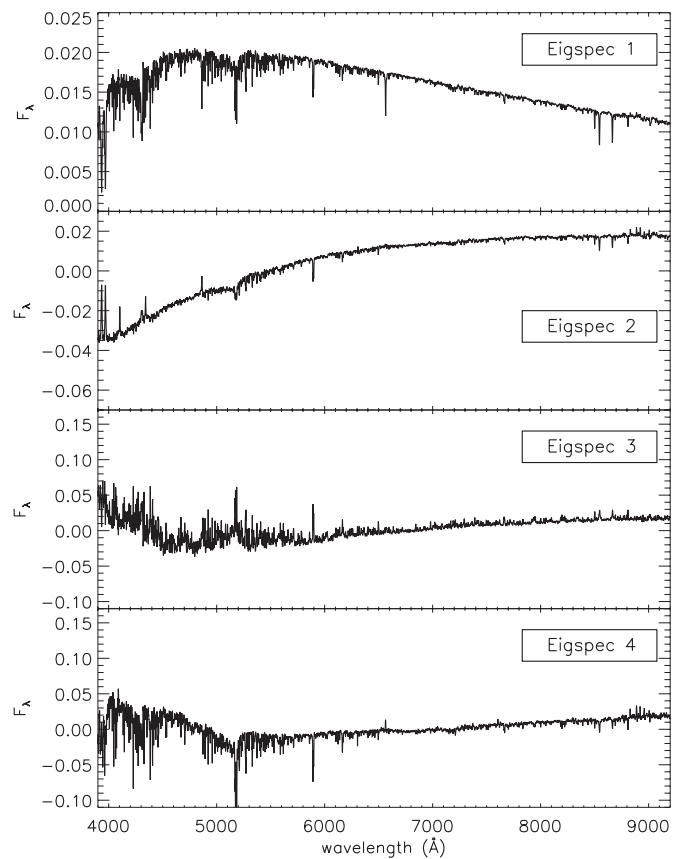


Figure 7. Four eigenspectra generated for the 5195 stars in bin 37 ($0.52 < g - r < 0.54$), plotted at vacuum wavelengths. The first eigenspectrum closely resembles a metal-rich ($[\text{Fe}/\text{H}] \sim -0.7$) dwarf. The variation of spectra in this bin is expected due to a high fraction of giant stars (which presumably also have lower metallicity than the majority of stars in the sample).

based on four and six eigenspectra is minor (a few percent or less over most of the wavelength range).

This is a much smaller number of eigencomponents than typically required. For example, Bailer-Jones et al. (1998) used the first 10 components to expand stellar spectra in their sample. The reason for this difference is that here we individually treat very narrow bins of the $g - r$ color. In order to describe spectral variations due to metallicity and gravity in each bin (i.e., at nearly a constant effective temperature), a large number of eigencomponents are not necessary. Figures 6 and 7 show the eigenspectra for bins 23 and 37, respectively (the spectra are plotted in vacuum wavelengths).

3. ANALYSIS OF PCA DECOMPOSITION RESULTS

3.1. Correlations Between Eigencoeficients and SSPP Parameters

For each $g - r$ bin, the ECs are expected to encode information about metallicity and gravity. Figures 8 and 9 demonstrate correlations between PCA ECs and SSPP metallicity and gravity for bins 23 and 37. For bin 23, a correlation between metallicity and EC2, EC3, and EC4 is present in the data, while there is no correlation with gravity. Note, however, that this bin includes only a small fraction of giant stars (3% with $\log(g) < 3$). For bin 37, ECs are correlated with both metallicity and gravity. However, as demonstrated in Figure 3, the metallicity and gravity are correlated for stars in this bin (due to SDSS spectroscopic target selection criteria, for more details see Yanny et al. 2009), and

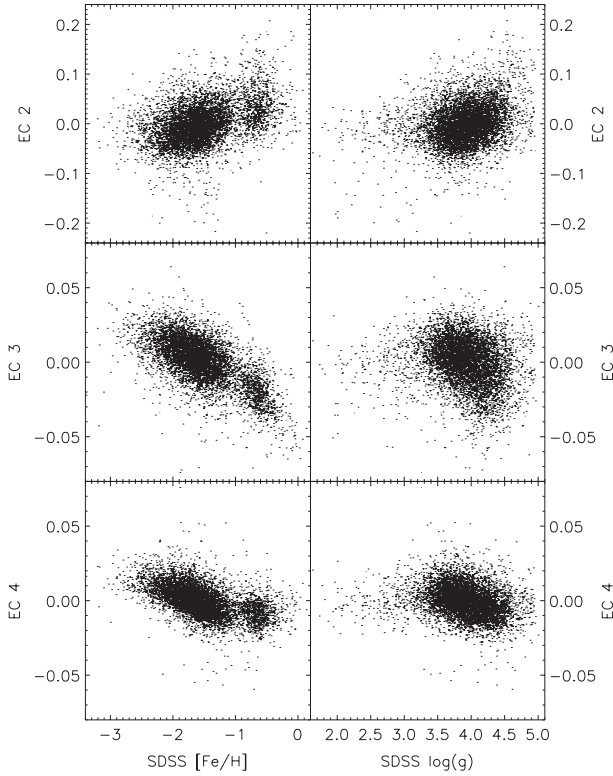


Figure 8. Eigencoeficients (ECs) for bin 23, corresponding to eigenspectra shown in Figure 6, shown as a function of metallicity (left column) and gravity (right column) computed by SSPP. Note a small fraction of giant stars ($\log(g) < 3$) and a correlation between metallicity and EC2, EC3, and EC4. The bimodal metallicity distribution reflects the SDSS targeting algorithm and significantly different metallicity distributions for halo ($[\text{Fe}/\text{H}] < -1$) and disk ($[\text{Fe}/\text{H}] > -1$) stars.

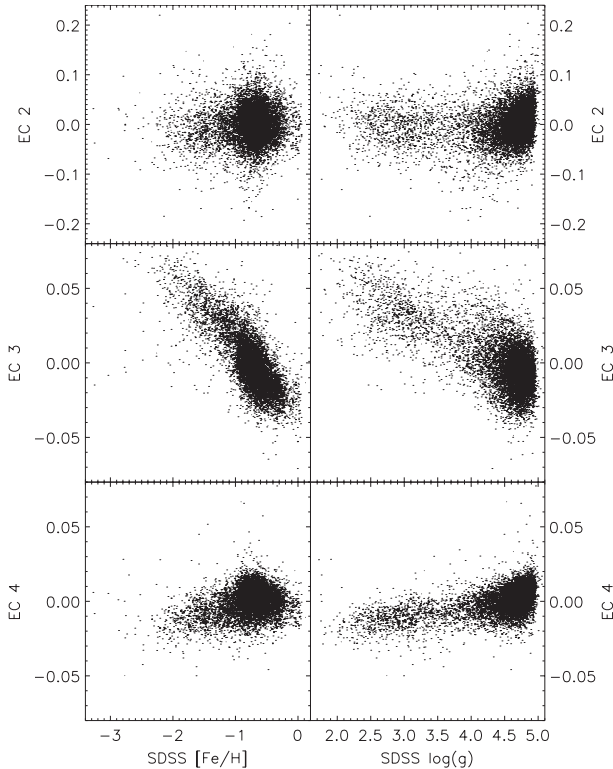


Figure 9. Eigencoeficients (ECs) for bin 37, corresponding to eigenspectra shown in Figure 7, shown as a function of metallicity (left column) and gravity (right column) computed by SSPP. Note a much larger fraction of giant stars than in Figure 8. The ECs seem correlated with both metallicity and gravity. The sample does not include high-metallicity giants.

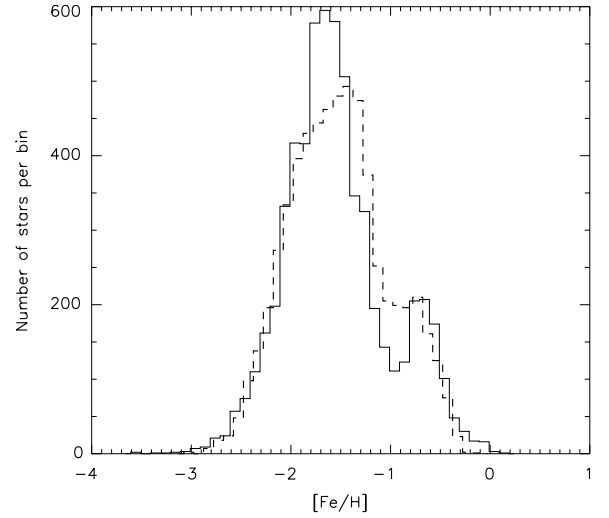


Figure 10. Comparison of the metallicity estimates obtained by the SDSS SSPP pipeline (solid histogram) and our PCA-based estimates (dashed histogram).

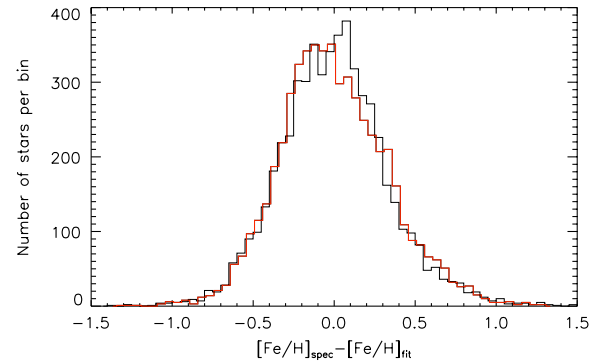
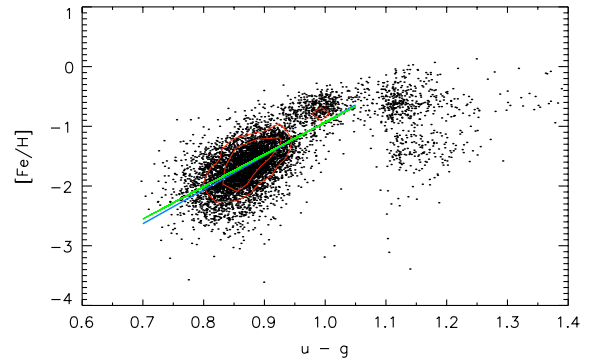


Figure 11. Independent test of two metallicity estimators based on a correlation of metallicity and the $u - g$ color. In the top plot, black points illustrate SSPP-measured metallicities, while the red contours illustrate our new metallicity measurements. The green and blue lines are the best-fit lines to the two data sets, respectively the SSPP fit and the new PCA fit. The bottom plot illustrates the scatter of each data set around the best-fit lines, with black being the SSPP data and red being the new metallicity data.

(A color version of this figure is available in the online journal.)

thus it is not clear which parameter drives the correlation with the ECs. A sample of high-metallicity giants or low-metallicity dwarfs is required to decouple the effects of these two parameters. Such stars are not present in the sample; the former are mostly nearby disk stars and thus too bright and saturated in SDSS data, while the latter are distant halo stars and too faint to be included in the SDSS spectroscopic survey (Ivezić et al. 2008b).

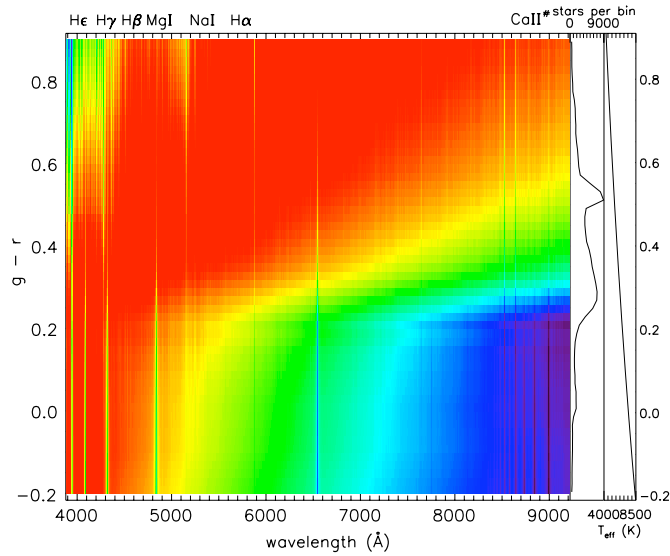


Figure 12. Progression of mean spectra (F_{λ}) plotted in vacuum wavelengths as a function of the $g-r$ color determined using PCA. The values increase logarithmically from blue to red. The two panels on the right side show the mean number of stars per 0.02 mag wide $g-r$ bin and the corresponding median effective temperature. A few spectral absorption lines are marked on top.

For a more quantitative investigation of the correlation observed in bin 23, we fit straight lines to the three relationships between metallicity and ECs 2, 3, and 4 (best-fit parabolas lead to the same conclusions). We then average the three best-fit metallicity estimates obtained using each EC and compare the result to values reported by the SSPP (Figure 10). The resulting

bimodal distributions look similar, though one could argue that the values determined with PCA have slightly larger random errors (by about 20%) than the official SDSS values because the distinction between the two peaks in metallicity distribution is somewhat erased.

For another comparison of the two metallicity estimators, we use the $u-g$ color obtained from imaging data. As shown by Ivezić et al. (2008b), for stars with blue $g-r$ colors, spectroscopic metallicity is strongly correlated with the $u-g$ color (see the top panel in Figure 11). They estimate that the random photometric metallicity errors are even smaller than the random metallicity errors determined by the SSPP from SDSS spectra (a random $u-g$ error of 0.02 mag induces a metallicity error in $[\text{Fe}/\text{H}]$ that varies from 0.02 dex at $[\text{Fe}/\text{H}] = -0.5$ to 0.11 dex at $[\text{Fe}/\text{H}] = -1.5$). Hence, for stars from bin 23, we can compare the spectroscopic metallicities determined by PCA and by the SSPP using the scatter around an average fit (see the bottom panel in Figure 11; a best-fit parabola leads to the same conclusion); the better metallicity determination would have less scatter. We find essentially identical error behavior, which suggests that the parameter precision obtained by PCA is comparable to that achieved by the SSPP for stars with $0.2 < g-r < 0.3$.

3.2. Mean Stellar Spectra Determined by PCA

One of the PCA products derived in this work is a set of high signal-to-noise gap-repaired mean spectra at each $g-r$ color. We show a stack of 55 such spectra in Figures 12 and 13. The variation of absorption line strengths and overall continuum shape with the $g-r$ color are easily discernible. For example, the depth of the $\text{H}\alpha$ line steadily decreases as the $g-r$ color becomes redder.

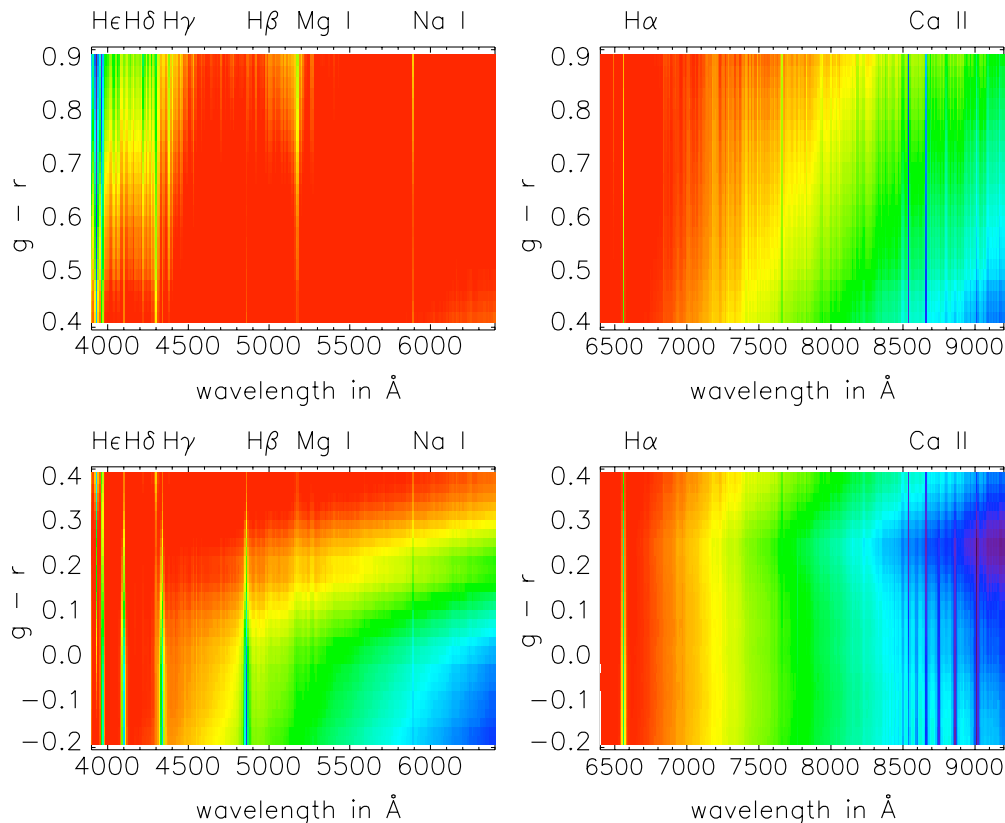


Figure 13. Analogous to Figure 12, except that the wavelength range and the $g-r$ range are split in halves, and each panel is separately color-coded to increase the contrast of spectral features.

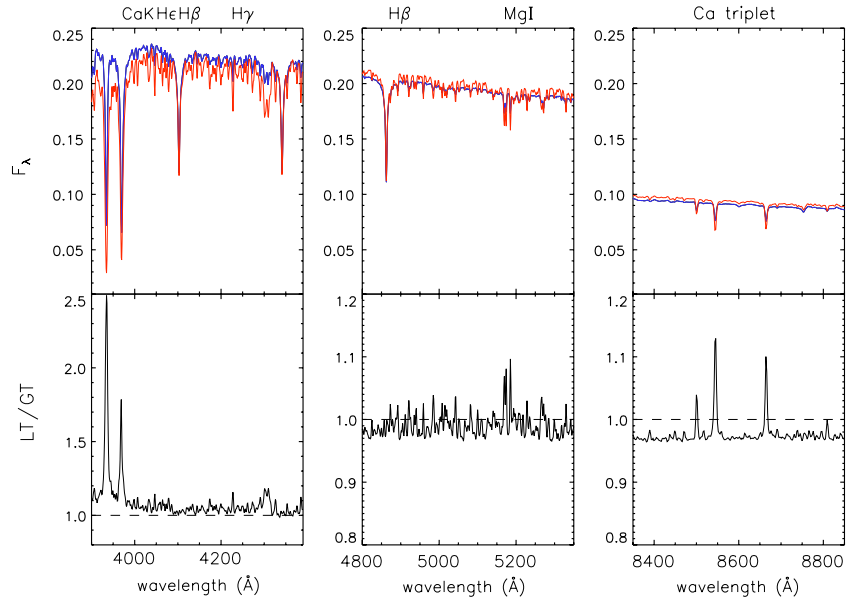


Figure 14. Top panels show two reconstructed spectra in three characteristic vacuum wavelength ranges for bin 23. The spectra are generated using mean ECs of the two clumps separated by $[\text{Fe}/\text{H}] = -1.05$ (see Figure 8; the blue line corresponds to the clump with $[\text{Fe}/\text{H}] < -1.05$ and the red line to the more metal-rich clump). Bottom panels show the ratio of the low-metallicity ($[\text{Fe}/\text{H}] \sim -1.5$) and the high-metallicity spectrum ($[\text{Fe}/\text{H}] \sim -0.6$).

(A color version of this figure is available in the online journal.)

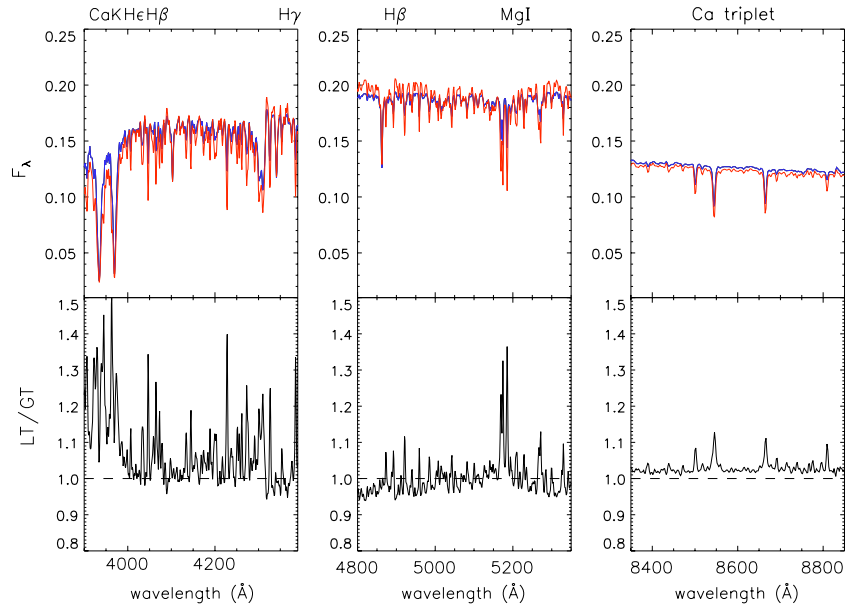


Figure 15. Similar to Figure 14, except that spectra are reconstructed for bin 37. The two reconstructed spectra are generated using mean ECs for the clump with $\log(g) < 3.7$ (blue line) and the clump with $\log(g) > 3.7$ (red line); see Figure 9 for the distribution of ECs.

(A color version of this figure is available in the online journal.)

In addition to mean spectra that roughly correspond to stars with *median* metallicity and gravity in a given $g-r$ bin, the remaining eigenspectra can be used to generate high signal-to-noise spectra for *any* combination of basic stellar parameters (effective temperature, metallicity, and gravity), within the parameter space probed by SDSS. Hence, given an arbitrary spectrum, one can attempt a low-dimensional fit using our library of eigenspectra, which we make publicly available.⁶

3.3. Variation of Mean Stellar Spectra with Metallicity and Gravity

The mean spectra shown in Figures 12 and 13 are averaged over metallicity and gravity distributions in the corresponding color bins. The small variations of stellar spectra with metallicity and gravity, at a fixed $g-r$ color, can be studied by drawing ECs from their observed distribution in a given bin. Given the quality of SDSS spectra and the high signal-to-noise ratio of the mean spectra (due to large number of stars per bin), these variations can be studied in great detail. An example of such a study is shown in Figures 14 and 15, where we contrast low- and

⁶ <http://www.astro.washington.edu/users/ivezic/rmcgirk/PCApublish.shtml>

high-metallicity stars from bin 23, and low (giants) and high (dwarfs) $\log(g)$ stars from bin 37. For example, the sensitivity of the Ca triplet (around ~ 8600 Å) to both metallicity and gravity is easily discernible (this wavelength range is exploited by the RAVE and Gaia surveys).

4. SUMMARY

We have applied PCA to $\sim 100,000$ stellar spectra obtained by the SDSS. After binning the sample using the $g-r$ color to study line variation at a nearly constant effective temperature as a function of metallicity and gravity, we find that the first four eigenspectra fully capture the observed spectral variations in each bin (within the noise in individual SDSS spectra). We analyze correlations between our PCA ECs and SSPP metallicity, and then use these correlations to measure metallicity. We find similar performance between the PCA-measured metallicity and the SSPP metallicity. This similarity suggests that random errors of SSPP parameters are just about as small as the signal-to-noise ratios of SDSS spectra allow.

We make publicly available the resulting high signal-to-noise mean spectra and the other three eigenspectra for all 55 color bins. These data can be used to generate high-quality spectra for an arbitrary combination of effective temperature, metallicity, and gravity, within the parameter space probed by SDSS. The utility of such spectra is wide and varied. Most obvious applications include searching for unusual spectra, training of various spectral classification methods, and color synthesis in arbitrary optical photometric systems, as well as various educational programs.

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